

# Quantum Cosmological Perturbations of Multiple Fluids

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The formalism to treat quantization and evolution of cosmological perturbations of multiple fluids is described. We first construct the Lagrangian for both the gravitational and matter parts, providing the necessary relevant variables and momenta leading to the quadratic Hamiltonian describing linear perturbations. The final Hamiltonian is obtained without assuming any equations of motions for the background variables. This general formalism is applied to the special case of two fluids, having in mind the usual radiation and matter mix which made most of our current Universe history. Quantization is achieved using an adiabatic expansion of the basis functions. This allows for an unambiguous definition of a vacuum state up to the given adiabatic order. Using this basis, we show that particle creation is well defined for a suitable choice of vacuum and canonical variables, so that the time evolution of the corresponding quantum fields is unitary. This provides constraints for setting initial conditions for an arbitrary number of fluids and background time evolution. We also show that the common choice of variables for quantization can lead to an ill-defined vacuum definition. Our formalism is not restricted to the case where the coupling between fields is small, but is only required to vary adiabatically with respect to the ultraviolet modes, thus paving the way to consistent descriptions of general models not restricted to single-field (or fluid).

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## I. INTRODUCTION

Cosmological perturbations are usually thought to originate from the short wavelength quantum vacuum fluctuations of the matter fields or fluids and the metric. The scales are subsequently increased to exit the Hubble radius, whence particles are produced, hopefully resulting in the observed spectrum of primordial perturbations. In inflationary models, the usual procedure consists in assuming a Friedmann-Lemaître-Robertson-Walker (FLRW) background metric with scale factor evolving following General Relativity (GR) Einstein equations sourced by a slowly rolling scalar field, leading to a quasiexponential, almost de Sitter inflation phase. Expanding the Einstein-Hilbert plus scalar field action to second order in perturbations, one then easily quantizes the so-called Mukhanov-Sasaki variable which can, for wavelengths much smaller than the Hubble scale, be postulated to initiate in a vacuum state: in a de Sitter universe, the (Bunch-Davies) vacuum state is unambiguously defined. The procedure can be extended to the quasi-de Sitter case that is of interest for inflation; this scheme is extremely well suited to the inflationary setup to which it is regularly applied.

In the alternative bouncing scenarios, primordial perturbations are set as vacuum initial conditions in the far past of the contracting phase, when the Universe is assumed almost flat for the scales of interest. When the contraction is dominated by a pressureless fluid, the spectrum of long wavelength perturbations is almost scale invariant [1–3] (and slightly blue). This is also the case for the so-called ekpyrotic scenarios [4–6]. In this case however, the bounce transition itself can lead essentially to any prediction [7].

Although the currently available data are well explained by single-field inflation, alternative views exist that should be considered. One might for instance be interested in investigating multifield inflation, although Bayesian analysis tend to disfavor them [8]. Indeed, additional fields are quite generic in supposedly realistic theories such those based on a grand unification or string theory, so that having more than one field present during the inflationary stage appears natural. Similarly, realistic bouncing models share the same characteristic, as one naturally expects several fluids, e.g. radiation and dust, to be present and active together with that responsible for the bouncing phase itself. A general rigorous formalism to deal with such situations is still lacking, although tentative options were proposed. In the multifield inflation scenario, it has been suggested to consider the coupling between fields as important only after the modes have entered the potential which, loosely speaking, is equivalent to becoming larger than the Hubble radius. It was also assumed that the coupling is present before

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potential entry, but is such that there exists a limit where it is asymptotically negligible, so that the vacuum can be defined as a combination of decoupled fields. These cases are discussed, e.g., in Refs. [9–18]. In both procedures the vacuum is set in the limit where the coupling is zero, a procedure which cannot take into account a possible divergent behavior of the couplings in the Ultraviolet (UV) limit. Such a behavior would lead to a set of ill-defined basis functions and, consequently, an ill-defined vacuum. To evaluate this behavior, one must calculate the next-to-leading-order corrections of all basis functions. The purpose of this work is precisely to calculate these corrections in a general way.

The present work, coming as a follow-up of Refs. [19–21], aims at partially closing the gap in providing this means, at least in cases consisting of many constituents, assumed uncoupled except through gravity. Our formalism henceforth permits us to set up initial conditions not only in an inflationary expanding universe, but also in a contracting universe, taking into account couplings between dust, radiation, and any other component that one might want to include in the model, under rather general circumstances. It is thus particularly suited to bouncing models in which the Universe starts big and filled with otherwise ordinary fluids.

In the following sections, we first set up the necessary formalism to describe cosmological perturbations around an FLRW background by expanding the Lagrangian action up to second order, assuming GR and an arbitrary number of fluids (Sec. II A); our formalism, based on canonical transformations, does not rely on the background satisfying Einstein equations, so that even with the Einstein-Hilbert action describing both background and perturbations, the actual background equations of motion are not necessarily the classical ones. Performing the required transformations, we deduce in Sec. II B the general Hamiltonian, then in Sec. II C we introduce the adiabatic/entropy mode splitting, which we illustrate with the special case of a two-component fluid, assumed barotropic. We find that coupling through gravity implies a special form of the coupling terms, which is quadratic in the fluid momenta.

The Hamiltonian is of course the starting point required for quantization, which we proceed with in Sec. III. Expanding the relevant variables in terms of harmonic functions of the Laplace-Beltrami operator, we derive the appropriate field operators and their momenta, and impose canonical quantization upon them. Because the Hamiltonian stems from perturbation theory and is thus quadratic, it turns out to be convenient to simplify the whole discussion using symplectic forms and a generic description of the Hamiltonian tensor in terms of block matrices describing the kinetic and potential terms. In Sec. III A, we present the quantization procedure valid for any system fitting this description and, in Sec. III B, we discuss the time evolution for such systems and the canonical transformations producing a set of variables where the quantization procedure leads to a unitary evo-

lution of the quantum fields. Finally, in Sec. III C, we obtain the explicit form for the adiabatic approximation for the basis functions. This permits the evaluation of the UV limit order by order in the adiabatic expansion. Using this tool, we show that, for the usual choice of variables, the adiabatic limit does not commute with the UV limit and consequently cannot be used to define a basis for the whole UV spectrum (which we call UV incomplete). On the other hand, using the variables introduced in this work, the vacuum is UV complete and the particle production is finite (in the sense that the particle density is finite). This result extends the work done in Ref. [21] (for particular examples, see also [22–33]) by showing a concrete example of choice of variables and initial conditions which leads to a unitary implementation of the time evolution for quantum fields interacting through a quadratic term in the Hamiltonian.

## II. SECOND ORDER CLASSICAL THEORY

Cosmological perturbations stem from an expansion around a FLRW background. The classical theory needs be written to second order in the perturbation variables, and subsequently quantized. In this section we first present the second order Lagrangian describing the dynamics of such linear cosmological perturbations of a FLRW universe with matter content provided by an arbitrary number of noninteracting fluids.

### A. Lagrangian formulation

Classical GR coupled to perfect fluids is most naturally expressed in terms of an action, deriving from a Lagrangian functional, from which the Hamiltonian formalism, necessary for quantization, can be derived. We begin by recalling the basics of the required Lagrangian formalism.

#### 1. Conventions

We consider a spacetime manifold described by a physical metric  $g_{\mu\nu}$ , with signature  $(-, +, +, +)$ . The torsion-free covariant derivative compatible with this metric is denoted by  $\nabla_\mu$ , such that  $\nabla_\mu g_{\alpha\beta} = 0$ .<sup>1</sup> We assume there exists a background FLRW metric  $\bar{g}_{\mu\nu}$  such that the difference  $g_{\mu\nu} - \bar{g}_{\mu\nu}$  can be seen as a “small perturbation” in the sense discussed in Ref. [34]. Accordingly, we define

<sup>1</sup> Our conventions for the curvature tensors are:

$$(\nabla_\mu \nabla_\nu - \nabla_\nu \nabla_\mu) v_\alpha = R_{\mu\nu\alpha}{}^\beta v_\beta, \quad R_{\mu\alpha} \equiv R_{\mu\nu\alpha}{}^\nu, \quad R \equiv R_\mu{}^\mu,$$

where  $v_\alpha$  is an arbitrary vector field.

the tensor  $\xi_{\mu\nu}$  and its contravariant form as

$$\xi_{\mu\nu} \equiv g_{\mu\nu} - \bar{g}_{\mu\nu}, \quad \xi^{\mu\nu} \equiv \bar{g}^{\mu\alpha} \bar{g}^{\nu\beta} \xi_{\alpha\beta}. \quad (1)$$

Here and in what follows, an overbar will always refer to a background quantity.

We now consider the case of a general space-time foliation defined by the normal timelike vector field  $u^\mu$  ( $u^\mu u_\mu = -1$ ), whose gradient can be decomposed into an extrinsic curvature  $\mathcal{K}_{\mu\nu}$  and an acceleration  $a_\mu \equiv u^\sigma \nabla_\sigma u_\mu$  through

$$\nabla_\mu u_\nu = \mathcal{K}_{\mu\nu} - n_\mu a_\nu. \quad (2)$$

The projector orthogonal to  $u^\mu$  (induced metric on the spatial hypersurfaces of the foliation) is given by

$$\gamma_{\mu\nu} = g_{\mu\nu} + u_\mu u_\nu.$$

Its action on an arbitrary tensor  $M_{\mu_1 \dots \mu_m}^{\nu_1 \dots \nu_k}$  is defined as

$$\gamma [M_{\mu_1 \dots \mu_m}^{\nu_1 \dots \nu_k}] \equiv \gamma_{\mu_1}^{\alpha_1} \dots \gamma_{\mu_m}^{\alpha_m} \gamma_{\beta_1}^{\nu_1} \dots \gamma_{\beta_k}^{\nu_k} M_{\alpha_1 \dots \alpha_m}^{\beta_1 \dots \beta_k},$$

thereby introducing the notation  $\gamma[\dots]$ , in terms of which the extrinsic curvature is simply found to be  $\mathcal{K}_{\mu\nu} \equiv \gamma[\nabla_\mu u_\nu]$ . The expansion factor  $\Theta$  and shear  $\sigma_{\mu\nu}$  are then given respectively by

$$\Theta \equiv \mathcal{K}_\mu^\mu \quad \text{and} \quad \sigma_{\mu\nu} \equiv \mathcal{K}_{\mu\nu} - \frac{1}{3} \Theta \gamma_{\mu\nu}. \quad (3)$$

An arbitrary tensor  $N_{\mu_1 \dots \mu_m}^{\nu_1 \dots \nu_k}$  will be called spatial if it is invariant under the projection, i.e., if it satisfies  $\gamma[N_{\mu_1 \dots \mu_m}^{\nu_1 \dots \nu_k}] = N_{\mu_1 \dots \mu_m}^{\nu_1 \dots \nu_k}$ . The covariant derivative compatible with the spatial metric  $\gamma_{\mu\nu}$  is

$$D_\alpha M_{\mu_1 \dots \mu_m}^{\nu_1 \dots \nu_k} \equiv \gamma[\nabla_\alpha M_{\mu_1 \dots \mu_m}^{\nu_1 \dots \nu_k}]. \quad (4)$$

This spatial covariant derivative defines the spatial Riemann curvature tensor  $\mathcal{R}_{\mu\nu\alpha}^\beta$  as

$$(D_\mu D_\nu - D_\nu D_\mu) A_\alpha \equiv \mathcal{R}_{\mu\nu\alpha}^\beta A_\beta, \quad (5)$$

where  $A_\beta = \gamma[A_\beta]$  is an arbitrary spatial vector field. The spatial Laplace operator is represented by the symbol  $D^2$ , i.e.,  $D^2 \equiv D_\mu D^\mu$ . In what follows, we shall denote the contraction with the normal vector field  $u^\mu$  with an index  $u$  (e.g.,  $M_{\alpha u} \equiv M_{\alpha\beta} u^\beta$ ).

The covariant derivative compatible with the background metric is represented by the symbol  $\bar{\nabla}$  or by a semicolon, i.e.,  $\bar{g}_{\mu\nu;\gamma} \equiv \bar{\nabla}_\gamma \bar{g}_{\mu\nu} = 0$ . Using a background foliation described by the normal vector field  $\bar{u}^\mu$ , we define the projector  $\bar{\gamma}_{\mu\nu}$ , spatial derivative  $\bar{D}_\mu$  and spatial Riemann tensor  $\bar{\mathcal{R}}_{\mu\nu\alpha}^\beta$ , as we have done for the objects derived from  $g_{\mu\nu}$ . We use the symbol “ $\parallel$ ” to represent the background spatial derivative, i.e.,  $\mathbf{T}_{\parallel\mu} \equiv \bar{D}_\mu \mathbf{T}$  for any tensor  $\mathbf{T}$ .

One should keep in mind that the background and perturbation tensors have their indices lowered and raised

always by the background metric. Finally, we define the dot operator of an arbitrary tensor as

$$\dot{M}_{\mu_1 \dots \mu_m}^{\nu_1 \dots \nu_k} \equiv \bar{\gamma} [\mathcal{L}_{\bar{u}} M_{\mu_1 \dots \mu_m}^{\nu_1 \dots \nu_k}], \quad (6)$$

where  $\mathcal{L}_{\bar{u}}$  is the Lie derivative in the direction of  $\bar{u}$ .

Specifying to the case of an FLRW background, the extrinsic curvature and the spatial Ricci tensor are diagonal and read

$$\bar{\mathcal{K}}_{\mu\nu} = \frac{1}{3} \bar{\Theta} \bar{\gamma}_{\mu\nu}, \quad \bar{\mathcal{R}}_{\mu\nu} = 2\bar{K} \bar{\gamma}_{\mu\nu},$$

with the expansion factor and the function  $\bar{K}$  being homogeneous, i.e.,  $\bar{\Theta}_{\parallel\mu} = 0 = \bar{K}_{\parallel\mu}$ . The expansion factor is simply proportional to the Hubble function  $H \equiv \frac{1}{3} \bar{\Theta}$ , itself giving the rate of time evolution of the scale factor  $a$ , namely  $H \equiv \dot{a}/a$ . Thus, the background Einstein tensor is given by

$$\bar{G}_{\mu\nu} = \left( 3\bar{K} + \frac{1}{3} \bar{\Theta}^2 \right) \bar{u}_\mu \bar{u}_\nu - \frac{1}{3} \left( 3\bar{K} + 2\dot{\bar{\Theta}} + \bar{\Theta}^2 \right) \bar{\gamma}_{\mu\nu}. \quad (7)$$

Having set the general notations, we now move to evaluate all the relevant perturbative contributions, namely those due to geometry and matter.

## 2. The geometric contribution

Let us define the “true” tensor [19]  $\mathcal{F}_{\mu\nu}^\alpha$  through the equation

$$\begin{aligned} (\nabla_\mu - \bar{\nabla}_\mu) A_\nu &= \mathcal{F}_{\mu\nu}^\beta A_\beta, \\ \mathcal{F}_{\alpha\beta}^\gamma &= -\frac{1}{2} g^{\gamma\sigma} (g_{\sigma\beta;\alpha} + g_{\sigma\alpha;\beta} - g_{\alpha\beta;\sigma}) \end{aligned} \quad (8)$$

(since the same coordinate system  $\{x^\mu\}$  is used for both the background and the perturbed geometries, the partial derivatives cancel out). With this tensor, we can now begin our evaluation of the geometric contribution to the second order action by noting that since the covariant derivative “ $;$ ” is with respect to the background metric, we have, to first order,

$$\mathcal{F}_{\alpha\beta\gamma} \approx -\frac{1}{2} (\xi_{\gamma\beta;\alpha} + \xi_{\gamma\alpha;\beta} - \xi_{\alpha\beta;\gamma}). \quad (9)$$

The perturbed Riemann tensor is related to the background Riemann tensor by the exact expression

$$R_{\mu\nu\alpha}^\beta = \bar{R}_{\mu\nu\alpha}^\beta + 2\mathcal{F}_{\alpha[\nu}^\beta{}_{;\mu]} + 2\mathcal{F}_{\alpha[\mu}^\gamma \mathcal{F}_{\nu]\gamma}^\beta, \quad (10)$$

where  $\bar{R}_{\mu\nu\alpha}^\beta$  is the Riemann tensor constructed with the background metric  $\bar{g}_{\mu\nu}$  and the brackets represent antisymmetrization over the indices bracketed. The expansion of the curvature scalar up to second order is therefore

$$\begin{aligned} R &\approx \bar{R} + \bar{R}_{\mu\nu} \xi^{\mu\nu} + (\xi^{\mu\nu}{}_{;\nu} - \xi^{;\mu}{}_{;\mu})_{;\mu} + \frac{1}{2} \xi_{;\mu}^\mu \left( \xi^{\mu\nu}{}_{;\nu} - \frac{1}{2} \xi^{;\mu}{}_{;\mu} \right) \\ &\quad - \mathcal{F}_{\mu\nu\alpha} \mathcal{F}^{\mu\alpha\nu} - \xi^{\mu\nu} \left( \frac{1}{2} \xi_{\nu;\mu} - \mathcal{F}_{\mu\nu}^\sigma{}_{;\sigma} \right), \end{aligned} \quad (11)$$

where again  $\bar{R}$  and  $\bar{R}_{\mu\alpha}$  are, respectively, the scalar curvature and the Ricci tensor of the background. To complete the expansion of the Lagrangian, we also need the metric determinant up to second order, namely

$$\sqrt{-g} \approx \sqrt{-\bar{g}} \left( 1 + \frac{1}{2}\xi - \frac{1}{4}\xi_{\mu\nu}\xi^{\mu\nu} + \frac{1}{8}\xi^2 \right). \quad (12)$$

Given the background foliation  $\bar{u}^\mu$ , the metric perturbation can be decomposed as

$$\xi_{\mu\nu} = 2\phi\bar{u}_\mu\bar{u}_\nu + 2B_{(\mu}\bar{u}_{\nu)} + 2C_{\mu\nu}, \quad (13)$$

where

$$\phi \equiv \frac{1}{2}\xi_{\bar{u}\bar{u}}, \quad B_\mu \equiv -\bar{\gamma}[\xi_{\bar{u}\mu}], \quad C_{\mu\nu} \equiv \frac{1}{2}\bar{\gamma}[\xi_{\mu\nu}].$$

Using the scalar, vector and tensor decomposition (see [35]), we rewrite the metric perturbations as

$$B_\mu = \mathcal{B}_{\parallel\mu} + \mathcal{B}_\mu, \\ C_{\mu\nu} = \psi\gamma_{\mu\nu} - \mathcal{E}_{\parallel\mu\nu} + \mathbf{F}_{(\nu\parallel\mu)} + W_{\mu\nu},$$

where  $\mathcal{B}^\mu_{\parallel\mu} = \mathbf{F}^\mu_{\parallel\mu} = W^\mu_{\parallel\mu} = W^\mu_{\parallel\nu} = 0$ . It is straightforward to show (see the Appendix A of Ref. [19]) that, in terms of this decomposition, the shear perturbation reads

$$\delta\sigma_{\mu\nu} = \left[ \bar{D}_{(\mu}\bar{D}_{\nu)} - \frac{\bar{\gamma}_{\mu\nu}\bar{D}^2}{3} \right] \delta\sigma^s + \delta\sigma^\nu_{(\nu\parallel\mu)} + \dot{W}_\mu{}^\alpha\bar{\gamma}_{\alpha\nu}, \quad (14)$$

where we have defined

$$\delta\sigma^s \equiv \left( \mathcal{B} - \dot{\mathcal{E}} + \frac{2}{3}\bar{\Theta}\mathcal{E} \right) \quad \text{and} \quad \delta\sigma^{\nu\alpha} \equiv \mathcal{B}^\alpha + \dot{\mathbf{F}}^\alpha. \quad (15)$$

The perturbation on the expansion factor gives

$$\delta\Theta = \bar{D}^2\delta\sigma^s + \bar{\Theta}\phi + 3\dot{\psi}. \quad (16)$$

Finally, the perturbations on the spatial Ricci tensor and curvature scalar are

$$\begin{aligned} \bar{\gamma}[\delta\mathcal{R}_\mu{}^{\bar{u}}] &= 0, \\ \bar{\gamma}[\delta\mathcal{R}_{\bar{u}}{}^\nu] &= -2\bar{K}(\mathcal{B}^{\parallel\nu} + \mathcal{B}^\nu), \\ \bar{\gamma}[\delta\mathcal{R}_\mu{}^\nu] &= -\psi_{\parallel\mu}{}^{\parallel\nu} - \bar{\gamma}_\mu{}^u(\bar{D}^2 + 4\bar{K})\psi \\ &\quad - (\bar{D}^2 - 2\bar{K})W_\mu{}^\nu, \\ \delta\mathcal{R} &= -4\bar{D}_K^2\psi, \end{aligned}$$

where we have defined the operator  $\bar{D}_K^2 \equiv \bar{D}^2 + 3\bar{K}$ .

After all these definitions, the general expression for the gravitational part of the second order Lagrangian is given by

$$\delta\mathcal{L}_g^{(2)} = \delta\mathcal{L}_g^{(2,s)} + \delta\mathcal{L}_g^{(2,v)} + \delta\mathcal{L}_g^{(2,t)} + \sqrt{-\bar{g}}l_g^{\text{bg}},$$

where the scalar part reads

$$\frac{\delta\mathcal{L}_g^{(2,s)}}{\sqrt{-\bar{g}}} = \frac{\bar{D}^2\delta\sigma^s\bar{D}_K^2\delta\sigma^s}{3\kappa} - \frac{\delta\Theta^2}{3\kappa} - 2\left(\frac{\psi}{2} - \phi\right)\frac{\bar{D}_K^2\psi}{\kappa}, \quad (17)$$

while the vector and tensorial sectors are, respectively

$$\frac{\delta\mathcal{L}_g^{(2,v)}}{\sqrt{-\bar{g}}} = \frac{\delta\sigma^\nu{}_{(\alpha\parallel\nu)}\delta\sigma^{\nu(\alpha\parallel\nu)}}{2\kappa}, \quad (18)$$

$$\frac{\delta\mathcal{L}_g^{(2,t)}}{\sqrt{-\bar{g}}} = \frac{\dot{W}_\nu{}^\gamma\dot{W}_\gamma{}^\nu + W_\mu{}^\nu(\bar{D}^2 - 2K)W_\nu{}^\mu}{2\kappa}, \quad (19)$$

as derived in Ref. [19]; note at this point that the quantities  $\dot{\phi}$  and  $\dot{\mathcal{B}}$  do not appear in the Lagrangian, having been transformed away through elimination of a total derivative term.

Finally the terms proportional to the background Einstein tensor read

$$2\kappa l_g^{\text{bg}} = \bar{G}_{\bar{u}\bar{u}}(B_\mu B^\mu - \phi^2 - 2\phi C) + \bar{G}_{\mu\nu}\bar{\gamma}^{\mu\nu}(2C^{\alpha\beta}C_{\alpha\beta} - C^2). \quad (20)$$

In what follows, after having written down the matter contribution to the second order action, we shall concentrate on the scalar parts of those, since it is the only contribution which has, so far unambiguously, been measured. Although the Lagrangian governing the scalar sector of the perturbations depends on the four field variables  $(\phi, \mathcal{B}, \psi, \mathcal{E})$ , it turns out to be more computationally efficient to write it in terms of the kinematic quantities  $\delta\Theta$ ,  $\delta\sigma$  and  $\delta\mathcal{R}$ , instead of directly in terms of the scalar variables above.

### 3. Matter part

The second order Lagrangian for the matter part consisting of a single generic fluid was also obtained in Ref. [19]. We consider a fluid having an energy density  $\bar{\rho}$ , pressure  $\bar{p}$  and associated sound velocity

$$\bar{c}_s^2 \equiv \frac{\partial\bar{p}}{\partial\bar{\rho}},$$

which is then perturbed so that the relevant variables will be the energy density perturbation  $\delta\rho$ , the pressure perturbation  $\delta p$ , and the velocity potential  $\mathcal{V}$  of the normalized velocity field of the fluid  $u_\mu$  defined through

$$u_\mu = \bar{u}_\mu - \phi\bar{u}_\mu + \mathcal{V}_{\parallel\mu}.$$

In general, there may also exist other relevant quantities, like an intrinsic entropy perturbation and other velocity potentials; here we will consider multiple noninteracting barotropic fluids. In this case, for each fluid, the intrinsic entropy perturbation and the other degrees of freedom decouple from the energy and pressure perturbations. We will therefore merely discard them.

We now assume a system consisting of  $N$  fluids, labeled by latin indices. As for the purely gravitational terms, the quantities  $\dot{\phi}$  and  $\dot{\mathcal{B}}$ , which appear in the original form of the Lagrangian, can be removed through elimination of another total derivative term [19]. This is possible for

each fluid term independently. The second order matter Lagrangian, according to Eq. (62) of Ref. [19], thus reads

$$\begin{aligned} \frac{\delta \mathcal{L}_{mi}^{(2)}}{\sqrt{-g}} = & \frac{\bar{c}_{si}^2 (\delta \rho_i^{gi})^2}{2(\bar{\rho}_i + \bar{p}_i)} + \frac{1}{2}(\bar{\rho}_i + \bar{p}_i) \mathcal{V}_i \bar{D}_K^2 \mathcal{V}_i \\ & - \frac{3\kappa}{4}(\bar{\rho}_i + \bar{p}_i)^2 \mathcal{V}_i^2 + (\bar{\rho}_i + \bar{p}_i) \delta \Theta \mathcal{V}_i + l_{mi}^{bg} \\ & - \frac{\bar{\rho}_i}{2} (B_\gamma B^\gamma - \phi^2 - 2C\phi) \\ & - \frac{\bar{p}_i}{2} (2C_\gamma{}^\nu C_\nu{}^\gamma - C^2), \end{aligned} \quad (21)$$

where the term  $l_{mi}^{bg}$  is given by

$$\begin{aligned} l_{mi}^{bg} = & -\frac{3}{4}(\bar{\rho}_i + \bar{p}_i) \mathcal{V}_i^2 (\bar{G}_{\bar{u}\bar{u}} - \kappa \bar{\rho}_i) \\ & - \frac{1}{4}(\bar{\rho}_i + \bar{p}_i) \mathcal{V}_i^2 (\bar{G}_{\mu\nu} \bar{\gamma}^{\mu\nu} - 3\kappa \bar{p}_i), \end{aligned} \quad (22)$$

and

$$\delta \rho_i^{gi} = \delta \rho_i - \bar{\Theta}(\bar{\rho}_i + \bar{p}_i) \mathcal{V}_i, \quad (23)$$

$$\delta \rho_i = -(\bar{\rho}_i + \bar{p}_i) \frac{\dot{\mathcal{V}}_i - \bar{c}_{si}^2 \bar{\Theta} \mathcal{V}_i - \phi}{\bar{c}_{si}^2}. \quad (24)$$

It is worth noting that in the case of a barotropic fluid set, each fluid introduces only one scalar field variable to the problem, namely  $\mathcal{V}_i$ , so that the whole matter Lagrangian depends on the set of variables  $\{\mathcal{V}_i\}_N$ . As in the gravitational sector case, it is more convenient to write the Lagrangian in terms of the relevant physical quantities. For each fluid, this is the energy density perturbation  $\delta \rho_i$  and its gauge-invariant version  $\delta \rho_i^{gi}$ . This is the only possible (apart from an irrelevant rescaling) gauge invariant combination that one can form using variables of the same fluid, namely  $\mathcal{V}_i$  and  $\dot{\mathcal{V}}_i$ .

Here we have discarded all terms proportional to the background equations for each fluid separately. This is possible because the fluids are not coupled, which means that the equation of motion for each fluid appears in the first order Lagrangian. Therefore, as explained in Ref. [19], we can remove such terms from the Lagrangian with a mere redefinition of the perturbation variables. This is done by modifying the second order by summing products of the first order variables. Since the first order Lagrangian appears as the product of the background equations of motion times the perturbations, this redefinition leaves the first order Lagrangian unmodified but introduces new second order terms in the Lagrangian, always multiplied by the zeroth order equations of motions, which are used to cancel out these unwanted terms. In the case at hand however, we are forced to keep the terms  $l_{mi}^{bg}$  because the Einstein equations appearing in the first order Lagrangian involve the total energy density and pressure, and not individual ones. For this reason, we

rewrite each  $l_{mi}^{bg}$  as

$$\begin{aligned} l_{mi}^{bg} = & \frac{3\kappa}{4}(\bar{\rho}_i + \bar{p}_i)^2 \mathcal{V}_i^2 - \frac{3\kappa}{4}(\bar{\rho}_i + \bar{p}_i)(\bar{\rho} + \bar{p}) \mathcal{V}_i^2 \\ & - \frac{3}{4}(\bar{\rho}_i + \bar{p}_i) \mathcal{V}_i^2 (\bar{G}_{\bar{u}\bar{u}} - \kappa \bar{\rho}) \\ & - \frac{1}{4}(\bar{\rho}_i + \bar{p}_i) \mathcal{V}_i^2 (\bar{G}_{\mu\nu} \bar{\gamma}^{\mu\nu} - 3\kappa \bar{p}), \end{aligned} \quad (25)$$

where the total energy density and pressure are,

$$\bar{\rho} = \sum_i \bar{\rho}_i, \quad \bar{p} = \sum_i \bar{p}_i, \quad (26)$$

and we note  $\kappa = 8\pi G_N = M_{\text{Plancck}}^{-2}$  (in units where  $\hbar = c = 1$ ). In Eq. (26) and the following, we assume all sums, unless explicitly stated otherwise, to run from 1 to  $N$ , the total number of fluids considered.

Now, we can remove the terms in the last two lines of Eq. (25) using the first order gravitational Lagrangian, and add the first line explicitly to the matter Lagrangian, yielding

$$\begin{aligned} \frac{\delta \mathcal{L}_{mi}^{(2)}}{\sqrt{-g}} = & \frac{\bar{c}_{si}^2 (\delta \rho_i^{gi})^2}{2(\bar{\rho}_i + \bar{p}_i)} + \frac{(\bar{\rho}_i + \bar{p}_i)}{2} \mathcal{V}_i \bar{D}_K^2 \mathcal{V}_i \\ & - \frac{3\kappa}{4}(\bar{\rho}_i + \bar{p}_i)(\bar{\rho} + \bar{p}) \mathcal{V}_i^2 + (\bar{\rho}_i + \bar{p}_i) \delta \Theta \mathcal{V}_i \\ & - \frac{\bar{\rho}_i}{2} (B_\gamma B^\gamma - \phi^2 - 2C\phi) \\ & - \frac{\bar{p}_i}{2} (2C_\gamma{}^\nu C_\nu{}^\gamma - C^2), \end{aligned} \quad (27)$$

so that the total Lagrangian will be given by the sum

$$\frac{\delta \mathcal{L}^{(2)}}{\sqrt{-g}} = \frac{\delta \mathcal{L}_g^{(2)}}{\sqrt{-g}} + \sum_i \frac{\delta \mathcal{L}_{mi}^{(2)}}{\sqrt{-g}}.$$

Using Eqs. (17) and (27), we obtain

$$\begin{aligned} \frac{\delta \mathcal{L}^{(2,s)}}{\sqrt{-g}} = & \frac{\bar{D}^2 \delta \sigma^s \bar{D}_K^2 \delta \sigma^s}{3\kappa} - \frac{\delta \Theta^2}{3\kappa} - 2(\psi - \phi) \frac{\bar{D}_K^2 \psi}{\kappa} \\ & + \sum_i \left[ \frac{\bar{c}_{si}^2 (\delta \rho_i^{gi})^2}{2(\bar{\rho}_i + \bar{p}_i)} + \frac{1}{2}(\bar{\rho}_i + \bar{p}_i) \mathcal{V}_i \bar{D}_K^2 \mathcal{V}_i \right] \\ & + \sum_i \left[ (\bar{\rho}_i + \bar{p}_i) \delta \Theta \mathcal{V}_i - \frac{3\kappa}{4}(\bar{\rho}_i + \bar{p}_i)(\bar{\rho} + \bar{p}) \mathcal{V}_i^2 \right], \end{aligned} \quad (28)$$

where we have again removed the terms linear in the background field equations using the first order Lagrangian.

Multiplying and dividing the term containing  $\delta \Theta^2$  by  $(\bar{\rho} + \bar{p})$ , and rewriting the numerator as a sum of  $(\bar{\rho}_i + \bar{p}_i)$ , we can combine it with the last line of the above,

obtaining

$$\begin{aligned} \frac{\delta \mathcal{L}^{(2,s)}}{\sqrt{-g}} &= \frac{\bar{D}^2 \delta \sigma^s \bar{D}_K^2 \delta \sigma^s}{3\kappa} + (2\phi - \psi) \frac{\bar{D}_K^2 \psi}{\kappa} \\ &+ \sum_i \left[ \frac{\bar{c}_{si}^2 (\delta \rho_i^{\text{gi}})^2}{2(\bar{\rho}_i + \bar{p}_i)} + \frac{1}{2} (\bar{\rho}_i + \bar{p}_i) \mathcal{V}_i \bar{D}_K^2 \mathcal{V}_i \right] \\ &- \frac{1}{3\kappa(\bar{\rho} + \bar{p})} \sum_i (\bar{\rho}_i + \bar{p}_i) \left[ \delta \Theta - \frac{3\kappa}{2} (\bar{\rho} + \bar{p}) \mathcal{V}_i \right]^2. \end{aligned} \quad (29)$$

It is convenient to work with gauge-invariant variables as e.g.,  $\delta \rho_i^{\text{gi}}$ , in terms of which we can express all other quantities. First, we define a gauge-invariant expansion factor

$$\Xi \equiv \delta \Theta - \frac{3\kappa}{2} (\bar{\rho} + \bar{p}) \mathcal{V} - 3 \frac{\bar{D}_K^2 \psi}{\Theta}, \quad (30)$$

where we introduced the total velocity potential  $\mathcal{V}$

$$\mathcal{V} \equiv \frac{1}{\bar{\rho} + \bar{p}} \sum_i (\bar{\rho}_i + \bar{p}_i) \mathcal{V}_i. \quad (31)$$

This potential represents the weighted average of the velocity potentials for each fluid using  $(\bar{\rho}_i + \bar{p}_i)$  as its weight.

Substituting this expression back into the total Lagrangian yields

$$\begin{aligned} \frac{\delta \mathcal{L}^{(2,s)}}{\sqrt{-g}} &= \frac{3\bar{D}^2 \Psi \bar{D}_K^2 \Psi}{\kappa \Theta^2} - \frac{\Xi^2}{3\kappa} + \sum_{i=1}^n \frac{\bar{c}_{si}^2 (\delta \rho_i^{\text{gi}})^2}{2(\bar{\rho}_i + \bar{p}_i)} \\ &- \sum_i \frac{9(\bar{\rho}_i + \bar{p}_i)}{2\Theta^2} \left[ \frac{3\kappa(\bar{\rho} + \bar{p})}{2} (\mathcal{U} - \mathcal{U}_i)^2 - \mathcal{U}_i \bar{D}_K^2 \mathcal{U}_i \right], \end{aligned} \quad (32)$$

where we have used the gauge-invariant variables

$$\mathcal{U}_i \equiv \psi + \frac{1}{3} \bar{\Theta} \mathcal{V}_i \quad \text{and} \quad \Psi \equiv \psi - \frac{1}{3} \bar{\Theta} \delta \sigma^s. \quad (33)$$

The variable  $\mathcal{U}$  is the weighted average of  $\mathcal{U}_i$ , analogous to  $\mathcal{V}$ . We have also removed a surface term and a linear term proportional to the background equations of motion, following what was done in Eq. (69) of Ref. [19]. Note that, in these variables, the Lagrangian in Eq. (32) naturally reduces to Eq. (69) of [19] when only a single fluid is present.

The final Lagrangian in Eq. (32) is organized as usual, the first  $2 + N$  kinematic terms involving the squares of the time derivatives and the last  $N$  terms the fluid potentials. It is a functional of the  $4 + N$  field variables  $(\phi, \mathcal{B}, \psi, \mathcal{E}, \{\mathcal{V}_i\}_N)$ . As was done for the individual matter and gravitational parts, here we also wrote the Lagrangian in term of physical quantities instead of directly in terms of these variables. This choice of variables simplifies the manipulation of the different terms in the Lagrangian (compare, for example, with the manipulations done in [36]). Nonetheless, the most important aspect of this form is the way it simplifies the constraints reduction as we see in the next section.

## B. Hamiltonian

The Hamiltonian formulation depends on the Legendre transform of the Lagrangian with respect to the field time derivatives. This transform is possible when the Hessian matrix is nonsingular, which is not the case here. For a singular Hessian one can use the Faddeev–Jackiw [37, 38] procedure. It starts by identifying the null-space of the Hessian matrix. The Lagrangian (32) depends on  $4 + N$  field variables and only on the time derivatives of  $2 + N$  variables, namely  $(\psi, \mathcal{E}, \{\mathcal{V}_i\}_N)$ . This allows an automatic identification of  $\phi$  and  $\mathcal{B}$  as part of the null-space of the Hessian matrix<sup>2</sup>. The time derivatives of  $\psi$  and  $\mathcal{E}$  are contained in  $\Psi$  and  $\Xi$  respectively through  $\delta \sigma^s$  and  $\delta \Theta$ . However,  $\delta \Theta$  depends on both  $\mathcal{E}$  and  $\psi$  while  $\delta \sigma^s$  depends only on  $\dot{\mathcal{E}}$  [see Eqs. (15) and (16)]. We can disentangle the two variables using, instead of  $\psi$ , the field

$$\psi^{\text{t}} \equiv \frac{C}{3} = \psi - \frac{\bar{D}^2 \mathcal{E}}{3}, \quad (34)$$

where  $C$  is the trace of the spatial projection of the metric perturbation in Eq. (13). In terms of this variable, the perturbation on the expansion rate then takes the simpler form

$$\delta \Theta = 3\dot{\psi}^{\text{t}} + \bar{D}^2 \mathcal{B} + \phi \bar{\Theta}.$$

Given the above, we are in a position to calculate the canonically conjugate momenta to  $\dot{\psi}^{\text{t}}$ ,  $\mathcal{E}$  and  $\dot{\mathcal{V}}_i$ . They read

$$\Pi_{\mathcal{V}_i} \equiv \frac{\partial \delta \mathcal{L}^{(2,s)}}{\partial \dot{\mathcal{V}}_i} = -\sqrt{-g} \delta \rho_i^{\text{gi}}, \quad (35)$$

$$\Pi_{\mathcal{E}} \equiv \frac{\partial \delta \mathcal{L}^{(2,s)}}{\partial \dot{\mathcal{E}}} = \frac{2\sqrt{-g}}{\kappa \bar{\Theta}} \bar{D}_K^2 \Psi, \quad (36)$$

$$\Pi_{\psi^{\text{t}}} \equiv \frac{\partial \delta \mathcal{L}^{(2,s)}}{\partial \dot{\psi}^{\text{t}}} = -2\sqrt{-g} \frac{\Xi}{\kappa}. \quad (37)$$

Since we arranged the Lagrangian (32) such that each kinematic term depends only on the time derivative of a single variable, each equation above relates one momentum with only one time derivative.

Solving the expressions (35–37) in terms of the time

<sup>2</sup> It is worth noting that the identification of the null-space is not straightforward as in a generic linear algebra problem. Any time dependent linear point transformation of the field variables generates additional terms depending on the time derivative of the transformation matrix.

derivatives, we obtain

$$\dot{\mathcal{V}}_i = \frac{\bar{c}_{si}^2 \Pi_{\mathcal{V}i}}{\sqrt{-\bar{g}}(\bar{\rho}_i + \bar{p}_i)} + \phi, \quad (38)$$

$$\mathcal{L}_{\bar{u}}(\bar{D}^2 \mathcal{E}) = \frac{3\kappa \bar{D}^2 \bar{D}_K^{-2} \Pi_{\mathcal{E}}}{2\sqrt{-\bar{g}}} - \frac{3\bar{D}^2 \psi}{\bar{\Theta}} + \bar{D}^2 \mathcal{B}, \quad (39)$$

$$\dot{\psi}^t = -\frac{\kappa \Pi_{\psi^t}}{6\sqrt{-\bar{g}}} + \frac{1}{2}\kappa(\bar{\rho} + \bar{p})\mathcal{V} + \frac{\bar{D}_K^2 \psi}{\bar{\Theta}} - \frac{\bar{\Theta}}{3}\phi - \frac{\bar{D}^2 \mathcal{B}}{3}, \quad (40)$$

and performing a Legendre transform in these variables then yields

$$\delta \mathcal{L}^{(2,s)} = \Pi_{\mathcal{E}} \mathcal{L}_{\bar{u}}(\bar{D}^2 \mathcal{E}) + \Pi_{\psi^t} \dot{\psi}^t + \sum_i \Pi_{\mathcal{V}i} \dot{\mathcal{V}}_i - \delta \mathcal{H}_c^{(2,s)}, \quad (41)$$

where

$$\begin{aligned} \delta \mathcal{H}_c^{(2,s)} = & \Pi_{\mathcal{E}} \mathcal{L}_{\bar{u}}(\bar{D}^2 \mathcal{E}) + \Pi_{\psi^t} \dot{\psi}^t + \sum_i \Pi_{\mathcal{V}i} \dot{\mathcal{V}}_i \\ & - \frac{3\kappa \Pi_{\mathcal{E}} \bar{D}^2 \bar{D}_K^{-2} \Pi_{\mathcal{E}}}{4\sqrt{-\bar{g}}} + \frac{\kappa \Pi_{\psi^t}^2}{12\sqrt{-\bar{g}}} - \sum_i \frac{\bar{c}_{si}^2 \Pi_{\mathcal{V}i}^2}{2\sqrt{-\bar{g}}(\bar{\rho}_i + \bar{p}_i)} \\ & + \sum_i \frac{9\sqrt{-\bar{g}}(\bar{\rho}_i + \bar{p}_i)}{2\bar{\Theta}^2} \left[ \frac{3\kappa(\bar{\rho} + \bar{p})}{2} (\mathcal{U} - \mathcal{U}_i)^2 - \mathcal{U}_i \bar{D}_K^2 \mathcal{U}_i \right], \end{aligned} \quad (42)$$

is the constrained Hamiltonian we are looking for, assuming time derivatives appearing in the first line to be given by Eqs. (38) – (40). Note that the Hamiltonian is a functional of the  $2N + 4$  dimensional phase space fields  $(\{\mathcal{V}_i, \Pi_{\mathcal{V}i}\}_N, \psi^t, \Pi_{\psi^t}, \mathcal{E}, \Pi_{\mathcal{E}})$ , and also depends on  $\phi$  and  $\mathcal{B}$ . However, this dependence is linear and only through the first three terms in the Hamiltonian (42) [see Eqs. (35)–(37)]. In other words,  $\phi$  and  $\mathcal{B}$  act as Lagrange multipliers so that variations of the Hamiltonian with respect to these variables provide the relevant constraints on the phase space.

Varying the Hamiltonian with respect to  $\phi$  and  $\mathcal{B}$  respectively yields

$$\frac{\partial \delta \mathcal{H}_c^{(2,s)}}{\partial \phi} = \sum_i \Pi_{\mathcal{V}i} - \frac{\bar{\Theta}}{3} \Pi_{\psi^t} = 0, \quad (43)$$

and

$$\frac{\partial \delta \mathcal{H}_c^{(2,s)}}{\partial \bar{D}^2 \mathcal{B}} = \Pi_{\mathcal{E}} - \frac{\Pi_{\psi^t}}{3} = 0. \quad (44)$$

These two equations reduce the number of momenta by two. We choose to express  $\Pi_{\psi^t}$  and  $\Pi_{\mathcal{E}}$  in terms of  $\{\Pi_{\mathcal{V}i}\}_N$ , which, applied to the kinematic part of the Lagrangian (41) represented by the first  $2 + N$  terms, yields

$$\delta \mathcal{L}^{(2,s)} = \sum_i \Pi_{\mathcal{V}i} \left( \frac{3}{\bar{\Theta}} \dot{\psi} + \dot{\mathcal{V}}_i \right) - \delta \mathcal{H}_c^{(2,s)},$$

and we are left with only  $N$  momenta. Given the Lagrangian structure, when we reduce the momenta

through linear constraints, the field variables containing time derivatives will also appear as some linear combination induced by the new momenta. In the equation above, the momenta multiply the gauge invariant variable  $\mathcal{U}_i$  [Eq. (33)]. Rewriting the terms in the parenthesis above generates new terms, which must be included in the final Hamiltonian, i.e.,

$$\delta \mathcal{L}^{(2,s)} = \sum_i \Pi_{\mathcal{U}i} \dot{\mathcal{U}}_i - \sum_i \frac{\dot{\bar{\Theta}}}{\bar{\Theta}} \Pi_{\mathcal{U}i} \mathcal{U}_i + \frac{\dot{\bar{\Theta}}}{\bar{\Theta}} \Pi_{\mathcal{U}} \psi - \delta \mathcal{H}_c^{(2,s)},$$

where we defined new momenta

$$\Pi_{\mathcal{U}i} \equiv \frac{3}{\bar{\Theta}} \Pi_{\mathcal{V}i},$$

and the total momentum

$$\Pi_{\mathcal{U}} \equiv \sum_i \Pi_{\mathcal{U}i}.$$

Finally, we can group the terms in the Lagrangian above and define the unconstrained Hamiltonian as

$$\delta \mathcal{H}^{(2,s)} \equiv \delta \mathcal{H}_c^{(2,s)} \Big|_{\substack{\Pi_{\psi^t} = \Pi_{\mathcal{U}} \\ \Pi_{\mathcal{E}} = \frac{1}{3} \Pi_{\mathcal{U}}}} + \sum_i \frac{\dot{\bar{\Theta}}}{\bar{\Theta}} \Pi_{\mathcal{U}i} \mathcal{U}_i - \frac{\dot{\bar{\Theta}}}{\bar{\Theta}} \Pi_{\mathcal{U}} \psi. \quad (45)$$

Arranging these terms we write the final Lagrangian and Hamiltonian explicitly

$$\delta \mathcal{L}^{(2,s)} = \sum_i \Pi_{\mathcal{U}i} \dot{\mathcal{U}}_i - \delta \mathcal{H}^{(2,s)}, \quad (46)$$

where the Hamiltonian, after removing another term proportional to a background equation, reads

$$\begin{aligned} \delta \mathcal{H}^{(2,s)} = & \sum_i \frac{\dot{\bar{\Theta}}}{\bar{\Theta}} \Pi_{\mathcal{U}i} \mathcal{U}_i + \frac{3\kappa(\bar{\rho} + \bar{p})}{2\bar{\Theta}} \mathcal{U} \Pi_{\mathcal{U}} \\ & + \sum_i \frac{\bar{c}_{si}^2 \bar{\Theta}^2 \Pi_{\mathcal{U}i}^2}{18\sqrt{-\bar{g}}(\bar{\rho}_i + \bar{p}_i)} - \frac{\kappa \bar{K} \Pi_{\mathcal{U}} \bar{D}_K^{-2} \Pi_{\mathcal{U}}}{4\sqrt{-\bar{g}}} \\ & + \sum_i \frac{9\sqrt{-\bar{g}}(\bar{\rho}_i + \bar{p}_i)}{2\bar{\Theta}^2} \left[ \frac{3\kappa(\bar{\rho} + \bar{p})}{2} (\mathcal{U} - \mathcal{U}_i)^2 - \mathcal{U}_i \bar{D}_K^2 \mathcal{U}_i \right]. \end{aligned} \quad (47)$$

The Lagrangian (46) shows that there are  $2N$  dynamical variables represented by the gauge invariant velocity potential and their momenta, i.e.,  $\{\mathcal{U}_i, \Pi_{\mathcal{U}i}\}_N$ . Naturally, the two scalar variables,  $\phi$  and  $\mathcal{B}$ , are absent from the unconstrained Hamiltonian (47). Since there are no momenta associated to  $\mathcal{E}$  and  $\psi$ , their appearance in the Hamiltonian would lead to new constraints, and indeed, they automatically cancel out.

This choice of variables satisfies the constraints and reduces the total number of variables to  $2N$ . Using the two constraints (43) and (44), we can recover the two momenta  $\Pi_{\mathcal{E}}$  and  $\Pi_{\psi^t}$ . Equations (39) and (40), relating the time derivatives and the momenta, can then be integrated to provide the values for the missing variables

$(\phi, \mathcal{B}, \mathcal{E}, \psi)$ . Naturally, one must also add two gauge conditions to completely fix this set of equations.

The form (47) decouples at leading order in the short wavelength limit. Despite this fact, it is however not as convenient, as will be shown explicitly in Sec. III, for the subsequent quantization, because particle creation, influenced by the next-to-leading order terms, leads to nonconvergent  $\beta$  functions. One could change variables directly to a more convenient set, but we present in the following section an intermediate step, thus introducing the equivalent, in the single-fluid case, of the Mukhanov-Sasaki variable. This step permits to write the Hamiltonian in a block-diagonal form.

### C. Adiabatic and Entropy Splitting

Our way of solving the constraints introduced new terms in the Hamiltonian (47), involving the total gauge invariant velocity potential and its momentum. These terms couple all dynamical variables. Varying the Hamiltonian with respect to  $\mathcal{U}_i$  or  $\Pi_{\mathcal{U}_i}$  yields terms proportional to  $\mathcal{U}$  and/or  $\Pi_{\mathcal{U}}$  which are related to the adiabatic modes of the perturbations. Thus, we can make a series of canonical transformations to rewrite the system in terms of adiabatic and entropy modes. In what follows, we perform these transformations, exhibit the adiabatic and entropy expansion for the general  $N$ -fluid case, and apply our result to the simpler (but natural) situation in which only two fluids, e.g. radiation and dust, are present.

#### 1. General case: $N$ fluids

First, we rewrite  $\{\mathcal{U}_i, \Pi_{\mathcal{U}_i}\}_N$  in terms of  $(\mathcal{U}, \Pi_{\mathcal{U}})$  and the relative variables

$$\tilde{\mathcal{U}}_i \equiv \mathcal{U}_i - \mathcal{U} \quad \text{and} \quad \tilde{\Pi}_{\mathcal{U}_i} \equiv \Pi_{\mathcal{U}_i} - \frac{(\bar{\rho}_i + \bar{p}_i)}{(\bar{\rho} + \bar{p})} \Pi_{\mathcal{U}}. \quad (48)$$

These variables are not independent since  $\sum_i \tilde{\Pi}_{\mathcal{U}_i} = 0$  and  $\sum_i (\bar{\rho}_i + \bar{p}_i) \tilde{\mathcal{U}}_i = 0$ . In terms of those, the total Lagrangian reads

$$\begin{aligned} \delta\mathcal{L}^{(2,s)} = & \sum_i \tilde{\Pi}_{\mathcal{U}_i} \dot{\tilde{\mathcal{U}}}_i + \Pi_{\mathcal{U}} \dot{\mathcal{U}} \\ & - \delta\mathcal{H}^{(2,s)} + \frac{\bar{\Theta}\Pi_{\mathcal{U}}}{\bar{\rho} + \bar{p}} \sum_i (\bar{\rho}_i + \bar{p}_i) \bar{c}_{si}^2 \tilde{\mathcal{U}}_i. \end{aligned} \quad (49)$$

Defining the total (weighted average) sound speed

$$\bar{c}_s^2 \equiv \frac{1}{\bar{\rho} + \bar{p}} \sum_i (\bar{\rho}_i + \bar{p}_i) \bar{c}_{si}^2, \quad (50)$$

and the new gauge-invariant variable  $\zeta$  (the usual curvature perturbation)

$$\zeta \equiv \mathcal{U} - \frac{\bar{K}\bar{\Theta}\bar{D}_K^{-2}\Pi_{\mathcal{U}}}{3\sqrt{-\bar{g}}(\bar{\rho} + \bar{p})}, \quad (51)$$

closely related to the Mukhanov-Sasaki variable, we can define a new Hamiltonian as

$$\delta\mathcal{H}_n^{(2,s)} \equiv \delta\mathcal{H}^{(2,s)} - \frac{\bar{\Theta}\Pi_{\mathcal{U}}}{\bar{\rho} + \bar{p}} \sum_i (\bar{\rho}_i + \bar{p}_i) \bar{c}_{si}^2 \tilde{\mathcal{U}}_i,$$

which is, explicitly

$$\begin{aligned} \delta\mathcal{H}_n^{(2,s)} = & -\frac{\kappa\bar{K}\Pi_{\mathcal{U}}\bar{D}_K^{-2}\Pi_{\mathcal{U}}}{4\sqrt{-\bar{g}}} - \frac{\bar{K}^2\Pi_{\mathcal{U}}\bar{D}_K^{-2}\Pi_{\mathcal{U}}}{2\sqrt{-\bar{g}}(\bar{\rho} + \bar{p})} \\ & + \frac{\bar{c}_s^2\bar{\Theta}^2\Pi_{\mathcal{U}}^2}{18\sqrt{-\bar{g}}(\bar{\rho} + \bar{p})} - \sqrt{-\bar{g}}\frac{9(\bar{\rho} + \bar{p})}{2\bar{\Theta}^2}\zeta\bar{D}_K^2\zeta \\ & + \sum_i \left\{ \frac{\bar{\Theta}}{\bar{\Theta}}\tilde{\Pi}_{\mathcal{U}_i}\tilde{\mathcal{U}}_i + \frac{27\sqrt{-\bar{g}}\kappa(\bar{\rho} + \bar{p})}{4\bar{\Theta}^2}(\bar{\rho}_i + \bar{p}_i)\tilde{\mathcal{U}}_i^2 \right. \\ & + \frac{\bar{c}_{si}^2\bar{\Theta}^2\tilde{\Pi}_{\mathcal{U}_i}^2}{18\sqrt{-\bar{g}}(\bar{\rho}_i + \bar{p}_i)} - \sqrt{-\bar{g}}\frac{9(\bar{\rho}_i + \bar{p}_i)}{2\bar{\Theta}^2}\tilde{\mathcal{U}}_i\bar{D}_K^2\tilde{\mathcal{U}}_i \\ & \left. - \frac{\bar{\Theta}\Pi_{\mathcal{U}}}{3(\bar{\rho} + \bar{p})}\bar{c}_{si}^2(\bar{\rho}_i + \bar{p}_i) \left[ 3\tilde{\mathcal{U}}_i - \frac{\bar{\Theta}\tilde{\Pi}_{\mathcal{U}_i}}{3\sqrt{-\bar{g}}(\bar{\rho}_i + \bar{p}_i)} \right] \right\}, \end{aligned} \quad (52)$$

in which yet another term proportional to the background equations of motion was removed. Finally, one can identify the term

$$\Pi_{\mathcal{U}}\mathcal{L}_{\bar{u}} \left[ \frac{\bar{K}\bar{\Theta}\bar{D}_K^{-2}\Pi_{\mathcal{U}}}{3\sqrt{-\bar{g}}(\bar{\rho} + \bar{p})} \right] \subset \delta\mathcal{H}_n^{(2,s)}$$

in the above, which can be combined with other terms to yield a total derivative that can subsequently safely be taken out. As a result, one finally arrives at the matter Lagrangian in the form of

$$\delta\mathcal{L}^{(2,s)} = \delta\mathcal{L}_a^{(2,s)} + \delta\mathcal{L}_s^{(2,s)}, \quad (53)$$

which represents the split, as expected: the first part,  $\delta\mathcal{L}_a^{(2,s)}$  is the usual Lagrangian for the adiabatic degree of freedom,

$$\delta\mathcal{L}_a^{(2,s)} = \Pi_{\zeta}\dot{\zeta} - \delta\mathcal{H}_a^{(2,s)}, \quad (54)$$

$$\delta\mathcal{H}_a^{(2,s)} = \frac{\bar{c}_s^2\bar{\Theta}^2\Pi_{\zeta}\bar{D}^2\bar{D}_K^{-2}\Pi_{\zeta}}{18\sqrt{-\bar{g}}(\bar{\rho} + \bar{p})} - \sqrt{-\bar{g}}\frac{9(\bar{\rho} + \bar{p})}{2\bar{\Theta}^2}\zeta\bar{D}_K^2\zeta, \quad (55)$$

where the momentum conjugate to  $\zeta$  is  $\Pi_{\zeta} \equiv \Pi_{\mathcal{U}}$ , while the entropy degrees of freedom are governed by the second part

$$\delta\mathcal{L}_s^{(2,s)} = \sum_i \tilde{\Pi}_{\mathcal{U}_i}\dot{\tilde{\mathcal{U}}}_i - \delta\mathcal{H}_s^{(2,s)}, \quad (56)$$

with the entropy Hamiltonian being

$$\begin{aligned} \delta\mathcal{H}_s^{(2,s)} = & \sum_i \left[ \frac{\bar{\Theta}}{\bar{\Theta}}\tilde{\Pi}_{\mathcal{U}_i}\tilde{\mathcal{U}}_i + \frac{27\sqrt{-\bar{g}}\kappa(\bar{\rho} + \bar{p})}{4\bar{\Theta}^2}(\bar{\rho}_i + \bar{p}_i)\tilde{\mathcal{U}}_i^2 \right. \\ & + \frac{\bar{c}_{si}^2\bar{\Theta}^2\tilde{\Pi}_{\mathcal{U}_i}^2}{18\sqrt{-\bar{g}}(\bar{\rho}_i + \bar{p}_i)} - \sqrt{-\bar{g}}\frac{9(\bar{\rho}_i + \bar{p}_i)}{2\bar{\Theta}^2}\tilde{\mathcal{U}}_i\bar{D}_K^2\tilde{\mathcal{U}}_i \\ & \left. - \frac{\bar{\Theta}\Pi_{\zeta}}{3(\bar{\rho} + \bar{p})}\bar{c}_{si}^2(\bar{\rho}_i + \bar{p}_i)\tilde{\delta}_{\psi i} \right], \end{aligned} \quad (57)$$



where we have defined the gauge-invariant energy density contrast

$$\delta_{\psi i} = 3\mathcal{U}_i - \frac{\bar{\Theta}\Pi_{\mathcal{U}_i}}{3\sqrt{-g}(\bar{\rho}_i + \bar{p}_i)} = \frac{\delta\rho_i}{\bar{\rho}_i + \bar{p}_i} + 3\psi, \quad (58)$$

and  $\delta\rho_i$  is given by Eq. (24). We can also define the variables

$$\delta_\psi = \frac{1}{(\bar{\rho} + \bar{p})} \sum_i (\bar{\rho}_i + \bar{p}_i) \delta_{\psi i} \quad \text{and} \quad \tilde{\delta}_{\psi i} = \delta_{\psi i} - \delta_\psi$$

for later convenience. Note that the only coupling with the adiabatic degree of freedom appears in the last line of the Hamiltonian (57).

Expressing the Lagrangian (56) as a function of  $\tilde{\delta}_{\psi i}$ , one gets

$$\delta\mathcal{L}_s^{(2,s)} = \sum_i \frac{3\sqrt{-g}(\bar{\rho}_i + \bar{p}_i)\tilde{\mathcal{U}}_i \dot{\tilde{\delta}}_{\psi i}}{\bar{\Theta}} - \delta\mathcal{H}_s^{(2,s)}, \quad (59)$$

where now

$$\begin{aligned} \delta\mathcal{H}_s^{(2,s)} = \sum_i & \left[ \frac{\sqrt{-g}\bar{c}_{si}^2(\bar{\rho}_i + \bar{p}_i)\tilde{\delta}_{\psi i}^2}{2} \right. \\ & - \sqrt{-g} \frac{9(\bar{\rho}_i + \bar{p}_i)}{2\bar{\Theta}^2} \tilde{\mathcal{U}}_i \bar{D}^2 \tilde{\mathcal{U}}_i \\ & \left. - \frac{\bar{\Theta}\Pi_\zeta}{3(\bar{\rho} + \bar{p})} \bar{c}_{si}^2(\bar{\rho}_i + \bar{p}_i)\tilde{\delta}_{\psi i} \right]. \end{aligned} \quad (60)$$

In the final Hamiltonian (60), we moved from the original variables  $\{\mathcal{U}_i, \Pi_{\mathcal{U}_i}\}$  to the adiabatic split involving the curvature perturbation  $\{\zeta, \Pi_\zeta\}$  and the entropy modes  $\{\tilde{\mathcal{U}}_i, \tilde{\Pi}_{\mathcal{U}_i}\}$ ; at this stage, it seems we have  $N + 1$  mode variables and momenta ( $N$  entropy and one adiabatic), although we started with  $N$ . This comes from the fact that we still have the constraints

$$\sum_i (\bar{\rho}_i + \bar{p}_i) \tilde{\mathcal{U}}_i = 0 = \sum_i (\bar{\rho}_i + \bar{p}_i) \tilde{\delta}_{\psi i} \quad (61)$$

to implement. Explicitly, we defined a set of new variables  $\tilde{P}_i \equiv -\tilde{\delta}_{\psi i}$  and  $\tilde{Q}_i \equiv 3\sqrt{-g}\bar{\Theta}^{-1}(\bar{\rho}_i + \bar{p}_i)\tilde{\mathcal{U}}_i$ , in terms of which the Lagrangian (59) reads

$$\delta\mathcal{L}_s^{(2,s)} = - \sum_i \tilde{Q}_i \dot{\tilde{P}}_i - \delta\mathcal{H}_s^{(2,s)} \rightarrow \sum_i \tilde{P}_i \dot{\tilde{Q}}_i - \delta\mathcal{H}_s^{(2,s)}, \quad (62)$$

where we have discarded the total derivative term. At this stage, one needs to set a reference fluid, indexed  $\ell$  say, with respect to which the relevant degrees of freedom will be defined. We thus define  $\tilde{P}_{i,\ell} \equiv \tilde{P}_i - \tilde{P}_\ell$ , leading to

$$\delta\mathcal{L}_s^{(2,s)} = \sum_{i \neq \ell} \tilde{P}_{i,\ell} \dot{\tilde{Q}}_i - \delta\mathcal{H}_s^{(2,s)}, \quad (63)$$

showing that, indeed, the actual number of degrees of freedom is  $N - 1$ .

Equations (61) permit us to rewrite the dependent variables  $\tilde{P}_\ell$  and  $\tilde{Q}_\ell$  in terms of the  $N - 1$  independent ones explicitly through

$$\tilde{P}_\ell = - \sum_{i \neq \ell} \frac{(\bar{\rho}_i + \bar{p}_i)}{(\bar{\rho} + \bar{p})} \tilde{P}_{i,\ell} \quad \text{and} \quad \tilde{Q}_\ell = - \sum_{i \neq \ell} \tilde{Q}_i. \quad (64)$$

The resulting total Hamiltonian, whose properties we discuss thoroughly in Sec. III B, includes (55) and

$$\begin{aligned} \delta\mathcal{H}_s^{(2,s)} = \sum_i & \left[ \frac{1}{2} \sqrt{-g} \bar{c}_{si}^2 (\bar{\rho}_i + \bar{p}_i) \tilde{P}_i^2 - \frac{\tilde{Q}_i \bar{D}^2 \tilde{Q}_i}{2\sqrt{-g}(\bar{\rho}_i + \bar{p}_i)} \right. \\ & \left. + \frac{\bar{\Theta}\Pi_\zeta}{3(\bar{\rho} + \bar{p})} \bar{c}_{si}^2 (\bar{\rho}_i + \bar{p}_i) \tilde{P}_i \right]; \end{aligned} \quad (65)$$

this Hamiltonian couples all the relevant field variables and all the corresponding momenta, without mixing the variables and the momenta, i.e. it does not include terms of the form  $\propto \tilde{Q}_i \tilde{P}_{j,\ell}$ , regardless of  $i$  and  $j$ , in contrast with our original Hamiltonian (47).

## 2. The 2-fluid case

We now consider the step discussed above for the special case of a two-fluid model for which no privileged fluid need be defined. In this case, a simple expansion in terms of one adiabatic ( $\{\zeta, \Pi_\zeta\}$ ) and one entropy ( $\{Q, P_Q\}$ ) mode is well-defined, which permits an easy writing of the Hamiltonian as well as, as it will turn out in Sec. III C, a natural way to set vacuum initial conditions.

Applying straightforwardly the scheme developed above, one sets  $\ell = 2$ , leading to the definition of the single momentum degree of freedom  $P_Q$  through

$$\begin{aligned} P_Q & \equiv \tilde{P}_{1,2} = \tilde{P}_1 - \tilde{P}_2 = \tilde{\delta}_{\psi 2} - \tilde{\delta}_{\psi 1} \\ & = \frac{\delta\rho_2}{(\bar{\rho}_2 + \bar{p}_2)} - \frac{\delta\rho_1}{(\bar{\rho}_1 + \bar{p}_1)} \end{aligned} \quad (66)$$

[see Eq. (58)], and the conjugate variable

$$Q \equiv \tilde{Q}_1 = \frac{3\sqrt{-g}}{\bar{\Theta}} \varpi (\mathcal{U}_1 - \mathcal{U}_2) \quad (67)$$

where

$$\varpi \equiv \frac{(\bar{\rho}_1 + \bar{p}_1)(\bar{\rho}_2 + \bar{p}_2)}{(\bar{\rho} + \bar{p})}. \quad (68)$$

The other relevant variables can all be expressed in terms of those above, namely

$$\tilde{P}_1 = \frac{(\bar{\rho}_2 + \bar{p}_2)}{(\bar{\rho} + \bar{p})} P_Q \quad \text{and} \quad \tilde{P}_2 = - \frac{(\bar{\rho}_1 + \bar{p}_1)}{(\bar{\rho} + \bar{p})} P_Q \quad (69)$$

and  $\tilde{Q}_2 = -\tilde{Q}_1 = -Q$ . Plugging these into Eq. (65) with  $N = 2$  leads to

$$\delta\mathcal{H}^{(2,s)} = \frac{1}{2} \sqrt{-g} \varpi \bar{c}_m^2 P_Q^2 - \frac{Q \hat{D}^2 Q}{\varpi \sqrt{-g} a^2} + \frac{\bar{c}_n^2 \varpi}{3(\bar{\rho} + \bar{p})} \Pi_\zeta P_Q, \quad (70)$$

where we have defined two different sound speeds

$$\bar{c}_m^2 \equiv \frac{\bar{c}_{s1}^2(\bar{\rho}_2 + \bar{p}_2) + \bar{c}_{s2}^2(\bar{\rho}_1 + \bar{p}_1)}{(\bar{\rho} + \bar{p})}, \quad (71)$$

$$\bar{c}_n^2 \equiv \bar{c}_{s1}^2 - \bar{c}_{s2}^2, \quad (72)$$

and the conformal Laplacian is  $\hat{D}^2 \equiv a^2 \bar{D}^2$ .

In order to add the adiabatic mode, we also define the operators  $\Delta_K \equiv \bar{D}^2 \bar{D}_K^{-2}$ , and  $\hat{D}_K^2 \equiv a^2 \bar{D}_K^2$ . The three operators  $\hat{D}^2$ ,  $\Delta_K$  and  $\hat{D}_K^2$  are time independent, i.e., the commutators

$$[\mathcal{L}_{\bar{u}}, \hat{D}^2] = [\mathcal{L}_{\bar{u}}, \hat{D}_K^2] = [\mathcal{L}_{\bar{u}}, \Delta_K] = 0$$

vanish when acting on any tensor field. In terms of these, the final Lagrangian reads

$$\delta \mathcal{L}^{(2,s)} = \Pi_\zeta \zeta' + P_Q Q' - \delta \mathcal{H}^{(2,s)}, \quad (73)$$

with Hamiltonian

$$\begin{aligned} \delta \mathcal{H}^{(2,s)} = & \Pi_\zeta \frac{1}{2m_\zeta} \Pi_\zeta + P_Q \frac{1}{2m_S} P_Q \\ & + \zeta \frac{m_\zeta \nu_\zeta^2}{2} \zeta + Q \frac{m_S \nu_S^2}{2} Q \\ & + \frac{\bar{c}_n^2}{\bar{c}_s^2 \bar{c}_m^2} \frac{\Pi_\zeta P_Q}{m_\zeta m_S \mathcal{N} H \Delta_K}, \end{aligned} \quad (74)$$

where we are using the Hubble function notation  $\bar{\Theta} = 3H$  and

$$m_\zeta \equiv \frac{a^3(\bar{\rho} + \bar{p})}{\mathcal{N} \bar{c}_s^2 \Delta_K H^2}, \quad \nu_\zeta^2 \equiv -\frac{\mathcal{N}^2 \bar{c}_s^2 \hat{D}^2}{a^2}, \quad (75)$$

$$m_S \equiv \frac{1}{\mathcal{N} a^3 \bar{c}_m^2 \varpi}, \quad \nu_S^2 \equiv -\frac{\mathcal{N}^2 \bar{c}_m^2 \hat{D}^2}{a^2}. \quad (76)$$

We have also performed a change in the time variable such that  $dt = \mathcal{N} d\tau$ , where  $t$  is cosmic time, and  $\mathcal{N}$  is an arbitrary lapse function. Examining the Lagrangian in Eq. (73), one notes that the first two terms will simply change as, for example,

$$dt \dot{\zeta} \rightarrow d\tau \zeta',$$

where a prime represents a derivative with respect to  $\tau$ , and the third term will be multiplied by the lapse function, i.e., the Hamiltonian part of the action is multiplied by  $\mathcal{N}$ . We have introduced the relevant  $\mathcal{N}$  factors directly on the definitions of the masses and frequencies above.

To conclude this part, one sees, on the canonical form of the Hamiltonian (74), that two uncoupled fluids in an FLRW universe end up being coupled through their interactions with the gravitational field, and the coupling term has a definite form: it is a momentum-momentum coupling whose amplitude is given by both sound velocities.

### III. QUANTIZATION OF MANY FIELDS WITH TIME-DEPENDENT QUADRATIC HAMILTONIANS

In this section we will present the main ingredients to perform the quantization of physical systems such as that presented in the previous section. For details about single component quantization, we refer the reader to Refs. [21] and Refs [39–43] for textbook treatments.

#### A. The general approach

Let us suppose a physical system having  $N$  different degrees of freedom

$$(\varphi_1, \varphi_2, \dots, \varphi_N),$$

the fields  $\varphi_i$  describing, for instance, the cosmological perturbations discussed above. We define a solution in the phase space as the vector

$$\chi_a = (\varphi_1, \dots, \varphi_N, \Pi_{\varphi_1}, \dots, \Pi_{\varphi_N}),$$

where  $\Pi_{\varphi_i}$  are the momenta canonically conjugate to  $\varphi_i$ . If the Hamiltonian is quadratic in the fields, we can write it in the form

$$\mathcal{H}(\chi) = \frac{1}{2} \chi_a \mathcal{H}^{ab} \chi_b, \quad (77)$$

where we introduced the symmetric Hamiltonian tensor  $\mathcal{H}^{ab}$ . In what follows, we shall also make use of the symplectic forms given by

$$\mathbb{S}_{ab} \equiv i \begin{pmatrix} 0 & \mathbb{1}_{N \times N} \\ -\mathbb{1}_{N \times N} & 0 \end{pmatrix}, \quad (78)$$

$$\mathbb{S}^{ab} \equiv i \begin{pmatrix} 0 & \mathbb{1}_{N \times N} \\ -\mathbb{1}_{N \times N} & 0 \end{pmatrix}, \quad (79)$$

with  $\mathbb{S}_{ac} \mathbb{S}^{cb} = \delta_a^b$ . The phase space indices are raised and lowered using the symplectic matrix, i.e.,

$$\chi^b \equiv \mathbb{S}^{ab} \chi_b, \quad \chi^{b*} \equiv \chi_a^* \mathbb{S}^{ab}. \quad (80)$$

The Hamiltonian equations for the system (77) above, usually written in the form

$$\dot{\varphi}_i = \frac{\partial \mathcal{H}}{\partial \Pi_{\varphi_i}} \quad \text{and} \quad \dot{\Pi}_{\varphi_i} = -\frac{\partial \mathcal{H}}{\partial \varphi_i},$$

then take the compact form

$$i \mathcal{L}_u \chi_a = \mathbb{S}_{ab} \mathcal{H}^{bc} \chi_c, \quad (81)$$

where  $u^\mu$  is the vector field which defines the foliation over which the Hamiltonian is built.

The product of two solutions  $\chi$  and  $\varpi$ , both assumed to satisfy (81), is defined as,

$$\mathbb{S}(\chi, \varpi) \equiv \int_\Sigma d^3x \chi_a \varpi_b \mathbb{S}^{ab}, \quad (82)$$

and it is conserved, i.e.,

$$i\mathcal{L}_u\mathbb{S}(\chi, \varpi) = 0, \quad (83)$$

by virtue of the Hamilton equation (81), the antisymmetry of  $\mathbb{S}$  and the symmetry of  $\mathcal{H}$ .

Let us now quantize the theory through canonical quantization rules, and consequently promote the fields to Hermitian operators. We will denote the field operators by hats over the corresponding classical field:  $\hat{\varphi}$  and  $\hat{\Pi}_\varphi$  will then be the field operators related to the classical variables  $\varphi$  and  $\Pi_\varphi$ , respectively. The canonical commutation relations which one then imposes to quantize the system can be regrouped in a single equation by means of the symplectic form  $\mathbb{S}$ , namely

$$[\hat{\chi}_a(\mathbf{x}), \hat{\chi}_b(\mathbf{y})] = \mathbb{S}_{ab}\delta^{(3)}(\mathbf{x} - \mathbf{y}) \quad (84)$$

(recall we work in units where  $\hbar = 1$ ).

We define the product of operators as

$$(\hat{\chi}, \hat{\gamma}) \equiv \mathbb{S}(\hat{\chi}^\dagger, \hat{\gamma}), \quad (85)$$

with  $X^\dagger$  the Hermitian conjugate of  $X$ ; this definition also implies

$$(\vartheta, v) = \int_{\Sigma} d^3x \vartheta_a^*(\mathbf{x}) \mathbb{S}^{ab} v_b(\mathbf{x}) \quad (86)$$

for ordinary phase space vectors  $\vartheta_a$  and  $v_a$ : taking the operators  $v\hat{I}$  and  $\vartheta\hat{I}$ , with  $\hat{I}$  is the identity operator, we can show that

$$\left[ (v\hat{I}, \hat{\chi}), (\vartheta\hat{I}, \hat{\chi}) \right] = \int_{\Sigma} d^3x \vartheta_a^*(\mathbf{x}) v_b^*(\mathbf{x}) \mathbb{S}^{ab} \hat{I} = (\vartheta, v^*) \hat{I}. \quad (87)$$

In what follows, we now assume any function to be associated naturally to an operator through the identity, and thus drop the  $\hat{I}$ .

Finally, we define the harmonic functions  $\mathcal{Y}_{\mathbf{k}}$  of the Laplace operator,

$$\bar{D}^2 \mathcal{Y}_{\mathbf{k}} = -\lambda_{\mathbf{k}}^2 \mathcal{Y}_{\mathbf{k}}, \quad \int_{\Sigma} d^3x \mathcal{Y}_{\mathbf{k}} \mathcal{Y}_{\mathbf{p}} = \delta^{(3)}(\mathbf{k} - \mathbf{p}), \quad (88)$$

where the index  $\mathbf{k}$  represents all the indices necessary to label the eigenvalues, and  $\delta^{(3)}(\mathbf{k} - \mathbf{p})$  represents the appropriate Dirac and Kronecker deltas. We have also chosen to work with real eigenfunctions of the Laplacian for simplicity (see [21] for a discussion about this point). It is convenient to define a phase space basis on  $\mathbf{k}$ -space (denoted with label  $\mathbf{k}$ ), i.e.,

$$U_{\mathbf{k},a}^i \equiv T_a^i(\mathbf{k}) \mathcal{Y}_{\mathbf{k}}, \quad (89)$$

where we have  $N$  complex phase space vectors  $T_a^i(\mathbf{k})$  or  $2N$  real ones, the number of real solutions matching the initial conditions degrees of freedom:  $N$  fields and  $N$  momenta. These solutions depend only on time ( $\bar{D}_\mu T_a^i = 0$ ) and the scale  $\mathbf{k}$ . These vectors represent a complete set of

solutions for the field equations and can thus be viewed as analogous to tetrads. They therefore carry a phase space index  $a$  as well as a solution index  $i$ ; there are as many solutions as there are degrees of freedom, i.e.,  $N$  complex or  $2N$  real solutions.

Given the definition (86), and the closure property (88), the product of two basis vectors will be given by

$$(U_{\mathbf{k}}^i, U_{\mathbf{p}}^j) = T_a^{i*}(\mathbf{k}) T_b^j(\mathbf{p}) \mathbb{S}^{ab} \delta^{(3)}(\mathbf{k} - \mathbf{p}), \quad (90)$$

by virtue of Eq. (88), so that, in order to have a normalized basis, we must impose that

$$T_a^{i*} T_b^j \mathbb{S}^{ab} = \delta^{ij}. \quad (91)$$

For these orthonormal solutions, the natural “metric” is simply the Kronecker delta  $\delta_{ij}$ , which we will use to raise and lower solution indices, i.e.,

$$T_{ia} \equiv \delta_{ij} T_a^j. \quad (92)$$

Given the orthonormal basis satisfying  $(U_{\mathbf{k}}^i, U_{\mathbf{p}}^j) = \delta^{ij} \delta^{(3)}(\mathbf{k} - \mathbf{p})$ , we can define the annihilation operators associated with this basis from the field operator  $\hat{\chi}$  as

$$\mathbf{a}_{\mathbf{k}}^i \equiv (U_{\mathbf{k}}^i, \hat{\chi}). \quad (93)$$

It follows directly from this definition and the properties above that

$$[\mathbf{a}_{\mathbf{k}}^i, \mathbf{a}_{\mathbf{p}}^{j\dagger}] = \delta^{ij} \delta^{(3)}(\mathbf{k} - \mathbf{p}). \quad (94)$$

We also want to impose  $[\mathbf{a}_{\mathbf{k}}^i, \mathbf{a}_{\mathbf{p}}^j] = 0 = [\mathbf{a}_{\mathbf{k}}^{i\dagger}, \mathbf{a}_{\mathbf{p}}^{j\dagger}]$ : this is equivalent to demanding that  $(U_{\mathbf{k}}^{i*}, U_{\mathbf{p}}^j) = 0$ . For our choice of basis functions in the form given in Eq. (89), one can see that the full set of conditions reduce to

$$T_a^{i*} T^{ja} = \delta^{ij}, \quad T_a^i T^{ja} = 0. \quad (95)$$

A closer look at the definition of  $\mathbf{a}_{\mathbf{k}}^i$  shows that

$$\mathbf{a}_{\mathbf{k}}^i = T_a^{i*} \int_{\Sigma} d^3x \mathcal{Y}_{\mathbf{k}}(\mathbf{x}) \hat{\chi}_a(\mathbf{x}) = T_a^{i*}(\mathbf{k}) \tilde{\chi}^a(\mathbf{k}), \quad (96)$$

where we have defined the transformed field  $\tilde{\chi}_a(\mathbf{k})$  of the field operator as

$$\tilde{\chi}_a(\mathbf{k}) \equiv \int_{\Sigma} d^3x \mathcal{Y}_{\mathbf{k}}(\mathbf{x}) \hat{\chi}_a(\mathbf{x}), \quad (97)$$

whose commutator reads

$$[\tilde{\chi}_a(\mathbf{k}), \tilde{\chi}_b(\mathbf{p})] = \mathbb{S}_{ab} \delta^{(3)}(\mathbf{k} - \mathbf{p}), \quad (98)$$

and in terms of which one can write down the associated creation operator through

$$\mathbf{a}_{\mathbf{k}}^{i\dagger} = -T_a^i(\mathbf{k}) \tilde{\chi}^a(\mathbf{k}). \quad (99)$$

The transformed field  $\tilde{\chi}_a(\mathbf{k})$  reduces to the usual Fourier transform when  $\mathcal{Y}_{\mathbf{k}} \propto e^{i\mathbf{k} \cdot \mathbf{x}}$ . This completes the quantum operator description of our Hamiltonian system.

## B. Vacuum evolution

Let us assume that we define a vacuum at the instant  $t_0$  using a given basis  $\mathbf{t}_a^i$  satisfying the conditions given in Eq. (95), i.e.,  $\mathbf{T}_a^i(t_0) = \mathbf{t}_a^i$ . At a later time  $t$ , we can decompose the vector  $\mathbf{T}_a^i(t)$  in terms of  $\mathbf{t}_a^i$  as

$$\mathbf{T}_a^i(t) = \alpha_{ij}^i(t) \mathbf{t}_a^j + \beta_{ij}^i(t) \mathbf{t}_a^{j*}, \quad (100)$$

where the functions

$$\alpha_{ij}^i(t) \equiv \mathbf{T}_a^i(t) \mathbf{t}_j^{a*} \quad \text{and} \quad \beta_{ij}^i(t) \equiv \mathbf{T}_a^i(t) \mathbf{t}_j^a \quad (101)$$

satisfy  $\alpha_{ij}^i(t_0) = \delta_{ij}^i$  and  $\beta_{ij}^i(t_0) = 0$ . Consequently, the annihilation and creation operators at  $t$  can be written in terms of the corresponding operators at  $t_0$  as

$$\begin{aligned} \mathbf{a}_{\mathbf{k}}^i(t) &= \alpha_{ij}^{i*}(t) \mathbf{a}_{\mathbf{k}}^j(t_0) - \beta_{ij}^{i*}(t) \mathbf{a}_{\mathbf{k}}^{j\dagger}(t_0), \\ \mathbf{a}_{\mathbf{k}}^{i\dagger}(t) &= \alpha_{ij}^i(t) \mathbf{a}_{\mathbf{k}}^{j\dagger}(t_0) - \beta_{ij}^i(t) \mathbf{a}_{\mathbf{k}}^j(t_0). \end{aligned} \quad (102)$$

It is clear from the equations above that if  $\beta_{ij}^i(t)$  vanishes, or equivalently if  $[\mathbf{a}_{\mathbf{k}}^i(t), \mathbf{a}_{\mathbf{p}}^j(t_0)] = 0$ , then both sets define the same vacuum. Writing the vacuum at a generic time  $t$  as  $|0_t\rangle$ , such that  $\mathbf{a}_{\mathbf{k}}^i(t) |0_t\rangle = 0$ , then the average number of particles at time  $t$  given by the number operator  $N_{\mathbf{k}}^i(t) \equiv \mathbf{a}_{\mathbf{k}}^{i\dagger}(t) \mathbf{a}_{\mathbf{k}}^i(t)$  which are present in the initial vacuum state  $|0_{t_0}\rangle$  reads

$$\langle 0_{t_0} | N_{\mathbf{k}}^i(t) | 0_{t_0} \rangle = \delta^{(3)}(\mathbf{0}) \int d^3k \sum_j |\beta_{ij}^i(t)|^2, \quad (103)$$

where the factor  $\delta^{(3)}(\mathbf{0}) \propto \mathcal{V}$  appears because we are calculating the number of particles in an infinite spatial section, with infinite volume  $\mathcal{V} \rightarrow \infty$ . Reference [21] provides a more detailed discussion about this infrared divergence in this context; the factor  $\delta^{(3)}(\mathbf{0})$  is the same as that appearing in usual QFT in which it is accounted for by considering a finite volume and taking the infinite volume limit at the very last step [44].

As reviewed in Ref. [21], in order for the quantum evolution to be unitary, the number operator average given by Eq. (103) must not diverge in the UV limit. Hamiltonians such as (74), containing interaction terms mixing momenta, can be problematic, because momenta exhibit a wavelength dependence  $\propto \lambda_{\mathbf{k}}^{1/2}$  initially, which can induce an UV divergence when such interaction terms become relevant for the dynamical evolution. In what follows, we present a formalism permitting to eliminate such terms and subsequently express the result in terms of Action-Angle (AA) variables, which will turn out to be more suitable for understanding the frequency behavior of the relevant degrees of freedom.

Consider a general Hamiltonian of the form  $H = \frac{1}{2} \chi_a H^{ab} \chi_b$  with the bilinear Hamiltonian tensor given by

$$H^{ab} = \begin{pmatrix} \mathbf{V} & \mathbf{0} \\ \mathbf{0} & \mathbf{T} \end{pmatrix}, \quad (104)$$

where  $\mathbf{V}$  and  $\mathbf{T}$  are arbitrary  $N \times N$  matrices. Our starting Hamiltonian tensor (104) assumes no mixing between coordinates and momenta. The Hamiltonian consisting of the sum of Eqs (55) and (65) is of the required form (104). Although not the most general bilinear form one may think of, it encompasses most of the cases relevant to cosmology, including the quite general situations discussed in [45], and therefore a thorough understanding of its properties provides an extremely useful first step. We can express its mixed form as

$$\mathcal{H}_a^b \equiv \mathcal{S}_{ac} \mathcal{H}^{cb} = \begin{pmatrix} 0 & i\mathbf{T} \\ -i\mathbf{V} & 0 \end{pmatrix}, \quad (105)$$

from which one can solve the eigenvalue problem<sup>3</sup>, namely

$$\mathcal{H}_a^c \Upsilon_c^j = \nu_j \Upsilon_a^j \quad \text{and} \quad \mathcal{H}_a^c \Upsilon_c^{j*} = -\nu_j \Upsilon_a^{j*}, \quad (106)$$

with  $j = 1, \dots, N$  denoting the eigenvalue number; unless otherwise explicitly stated, there is no summation on the eigenvalue number  $j$ . It is worth noting that  $\mathcal{H}_a^c$  is a self-adjoint operator with respect to the product, i.e.,

$$\begin{aligned} (\chi, \mathcal{H} \cdot \vartheta) &= (\mathcal{H} \cdot \chi, \vartheta), \\ (\mathcal{H} \cdot \chi)_a &\equiv \mathcal{H}_a^b \chi_b. \end{aligned} \quad (107)$$

In this case, the eigenvalues are real and the basis can be made orthonormal.

Equations (106) show that there are  $N$  eigenvectors with eigenvalues  $\nu_j$ , their complex conjugate having eigenvalues  $-\nu_j$ . These eigenvectors can be written explicitly as (we assume  $\mathbf{T}$  to be invertible, which is always the case in our context)

$$\Upsilon_a^j \doteq \left( \frac{q^j}{\sqrt{2\nu_j}}, -i\sqrt{\frac{\nu_j}{2}} \mathbf{T}^{-1} q^j \right), \quad (108)$$

where  $q^j$  satisfies

$$\mathbf{T} \mathbf{V} q^j = \nu_j^2 q^j, \quad (109)$$

and we have chosen  $\nu_j > 0$ . Also, one should keep in mind that  $\mathbf{T}$  is an  $N \times N$  matrix and each  $q^j$  an  $N$  vector in configuration space, so  $\Upsilon^j$  is a  $2N$  vector in phase space. Expressed explicitly in components, the  $q^j$  can be chosen in order to yield

$$\Upsilon_a^{i*} \mathcal{S}^{ab} \Upsilon_b^j = \delta^{ij}. \quad (110)$$

It is now possible to construct a real basis for vectors as

$$Q^{ja} = \frac{\Upsilon^{ja} + \Upsilon^{ja*}}{\sqrt{2m_j \nu_j}} = \left( \frac{1}{\sqrt{m_j}} \mathbf{T}^{-1} q^j, 0 \right) \quad (111)$$

<sup>3</sup> We assume wavelengths small enough compared to any relevant length scale of the system to ensure that this eigenvalue problem makes sense.

and

$$\Pi^{ja} = i\sqrt{\frac{m_j \nu_j}{2}} (\Upsilon^{ja} - \Upsilon^{ja*}) = (0, \sqrt{m_j} q^j), \quad (112)$$

in which we introduced arbitrary functions of time  $m_j$ ; we will later use the freedom to choose these functions at will to deduce the meaningful variables for which the time evolution of the quantum field operators can be made unitary.

It is possible to expand the matrix  $\mathbb{S}$  on either basis, namely

$$\mathbb{S}^{ab} = \sum_j (\Upsilon^{ja} \Upsilon^{jb*} - \Upsilon^{ja*} \Upsilon^{jb}) \quad (113)$$

or

$$\mathbb{S}^{ab} = i \sum_j (Q^{ja} \Pi^{jb} - \Pi^{ja} Q^{jb}), \quad (114)$$

and the Hamiltonian tensor as

$$H^{ab} = \sum_j \nu_j (\Upsilon^{ja} \Upsilon^{jb*} + \Upsilon^{ja*} \Upsilon^{jb}). \quad (115)$$

Now, defining the canonical variables

$$Q^j \equiv \chi_a Q^{ja} \quad \text{and} \quad \Pi^j \equiv \chi_a \Pi^{ja}, \quad (116)$$

one finds that the Lagrangian

$$\mathcal{L} = \frac{i}{2} \chi_a \mathbb{S}^{ab} \dot{\chi}_b - \frac{1}{2} \chi_a H^{ab} \chi_b \quad (117)$$

reduces to

$$\begin{aligned} \mathcal{L} = & \sum_j \frac{1}{2} (\Pi^j \dot{Q}^j - \dot{\Pi}^j Q^j) \\ & - \left[ \sum_i \frac{\Pi^{i2}}{2m_i} + \frac{1}{2} m_i \nu_i^2 Q^{i2} + \sum_{i,j} \Pi^i \mathcal{M}^{ij} Q^j \right], \end{aligned} \quad (118)$$

where the matrix  $\mathcal{M}^{ij}$  is defined through the time evolution of the canonical variable  $Q^j$ , namely

$$\dot{Q}^{ja} = \sum_i \mathcal{M}^{ij} Q^{ia}. \quad (119)$$

Similarly, one could define the matrix  $\mathcal{N}^{ij}$  for the time evolution of the momentum through

$$\dot{\Pi}^{ja} = \sum_i \mathcal{N}^{ij} \Pi^{ia}. \quad (120)$$

Using that  $Q^{ia} \Pi_a^j = i\delta^{ij}$  and its time derivative, one however finds that  $\mathcal{M}^{ij} + \mathcal{N}^{ij} = 0$ , so one really only requires knowledge of the matrix  $\mathcal{M}^{ij}$ .

The Hamiltonian appearing in the second line of Eq. (118) does not contain quadratic terms mixing the momenta. This is not enough however: interacting terms of the form  $Q^i Q^j$  are those whose UV limit behavior is

under control, since they always lead to an  $\lambda_k^{-1/2}$  power as leading term initially. Cross-terms mixing the momentum and coordinate of the same degree of freedom can be problematic however, and we need to perform a further canonical transformation in order to eliminate all symmetric mixing terms involving momenta. The transformation

$$\begin{cases} \Pi^i = P^i + \sum_j \mathcal{R}^{ij} Q^j, \\ \bar{Q}^i = Q^i, \end{cases} \quad (121)$$

which is canonical if and only if  $\mathcal{R}^{ij} = \mathcal{R}^{ji}$ , permits to achieve the goals discussed above (from here on we drop the overbar in the field variable  $\bar{Q}^i$ ). The Hamiltonian then reads

$$\begin{aligned} \mathcal{H} = & \sum_{i,j} \left\{ \frac{P^{i2}}{2m_i} + P^i \mathcal{M}^{ij} Q^j + \frac{P^i \mathcal{R}^{ij} Q^j}{m_i} + \frac{Q^i Q^j}{2} \times \right. \\ & \left. \times \left[ m_i \nu_i^2 \delta^{ij} + \dot{\mathcal{R}}^{ij} + \sum_l \left( \frac{\mathcal{R}^{il} \mathcal{R}^{lj}}{m_l} + 2\mathcal{R}^{il} \mathcal{M}^{lj} \right) \right] \right\}. \end{aligned} \quad (122)$$

The symmetry condition  $\mathcal{R}^{ij} = \mathcal{R}^{ji}$  is highly nontrivial since it actually imposes additional constraints unfortunately preventing a full removal of the unwanted terms. In Eq. (122) for instance, it would be the term containing  $\mathcal{M}^{ij}$ , and the latter matrix is not necessarily symmetric, and so cannot be fully canceled by the following term containing  $\mathcal{R}^{ij}$ . Hence, another step is required: defining

$$\mathcal{B}^{ij} \equiv 2 \frac{m_i \nu_i}{\nu_i + \nu_j} \mathcal{M}^{ij} = \mathcal{B}^{(ij)} + \mathcal{B}^{[ij]}, \quad (123)$$

one can choose the canonical transformation by imposing

$$\mathcal{R}^{ij} = -\mathcal{B}^{(ij)}, \quad (124)$$

yielding

$$\mathcal{H} = \sum_i \left( \frac{P^{i2}}{2m_i} + \frac{m_i \nu_i^2 Q^{i2}}{2} \right) + \sum_{i,j} \left( \frac{P^i \tau^{ij}}{2m_i \nu_i} - \frac{Q^i \gamma^{ij}}{2} \right) Q^j, \quad (125)$$

where

$$\gamma^{ij} \equiv \sum_l \left[ \frac{\mathcal{B}^{(il)} \mathcal{B}^{(lj)} \nu_j}{m_l \nu_l} + \frac{\mathcal{B}^{(il)} \mathcal{B}^{[lj]} (\nu_l + \nu_j)}{m_l \nu_l} \right] + \dot{\mathcal{B}}^{(ij)}, \quad (126)$$

$$\tau^{ij} \equiv \left[ \mathcal{B}^{[ij]} (\nu_i + \nu_j) - \mathcal{B}^{(ij)} (\nu_i - \nu_j) \right], \quad (127)$$

with  $\tau^{ji} = -\tau^{ij}$ . The matrices  $\gamma^{ij}$  and  $\tau^{ij}$  are the effective couplings between the various fluids. In the single-fluid case, one often defines an effective time-dependent frequency  $\bar{\nu}$ , which could be generalized in the multiple fluid case through

$$\bar{\nu}_i^2 = \nu_i^2 - \frac{\gamma^{ii}}{m_i}. \quad (128)$$

In the usual single-fluid case, Eq. (128) becomes

$$\bar{\nu} = \nu - \left( \frac{\mathcal{B}^2}{m^2} + \frac{\dot{\mathcal{B}}}{m} \right),$$

which reduces to the effective potential  $z''/z$  of Ref. [36] when one chooses  $m \rightarrow 1$ . In the case at hand however, there are two extra terms that have to be taken care of.

Our final form (125) could have been directly obtained with a direct canonical transformation from Eq. (47) instead of going through the steps leading to Eqs. (55) and (65); it turns out that the adiabatic and entropy split can be useful to compare with other formalisms, since it makes apparent the usual Mukhanov-Sasaki variable. Besides, it allows for an easy subsequent diagonalization since it sets the Hamiltonian in the block diagonal form (104).

The single term mixing coordinates and momenta in the Hamiltonian (125),  $\tau^{ij}$ , being antisymmetric, can only relate the momentum of a given fluid to the field variable of all other fields but itself. As we anticipated above and will see below, the influence of such kind of terms on the dynamics keeps the degrees of freedom well-behaved in the UV limit.

The coupling  $\gamma^{ij}$  enters through a symmetric term, and one can therefore restrict attention to  $\gamma^{(ij)}$ . Usually, one incorporates its diagonal part into the effective mass, as in Eq. (128), leaving only a pure “self-coupling” term. Here, we shall keep this term as it appears in Eq. (125) to prove that its presence does not change the fact that the UV behavior still leads to convergent  $\beta$  functions, hence rendering possible a complete definition of a vacuum state. For this to be true, one needs to choose wisely the otherwise arbitrary functions  $m_i$  to remove any potentially problematic  $\lambda_{\mathbf{k}}$ -behavior. This is what we can see explicitly by going to the Action-Angle variables  $I_i$  and  $\theta_i$ .

The AA variables are defined through

$$Q_i = \sqrt{\frac{2I_i}{m_i\nu_i}} \sin \theta_i \quad \text{and} \quad P_i = \sqrt{2I_i m_i \nu_i} \cos \theta_i, \quad (129)$$

the functions  $I_i$  being the momenta associated to the coordinates  $\theta_i$ . It is worth mentioning that at this point we used the original frequency  $\nu_i$  instead of  $\bar{\nu}_i$  (as was used in [21]) in the implicit definition of  $I_i$  and  $\theta_i$  above. This choice will result in a slightly different approximation, but an equivalent scheme. Its usefulness arises from the simplicity of the coupling terms in Eq. (130) which would be spoiled by factors of  $\nu_i/\bar{\nu}_j$ .

The canonical variables (129) allow us to express the Hamiltonian in the required form, namely

$$\begin{aligned} \mathcal{H} = & \sum_i I_i [\nu_i + \dot{\alpha}_i \sin(2\theta_i)] \\ & - \sum_{i,j} \sqrt{I_i I_j} \left[ \sin \theta_i \sin \theta_j \bar{\gamma}^{ij} + \frac{\sin(\theta_i - \theta_j) \bar{\tau}^{ij}}{2} \right], \end{aligned} \quad (130)$$

where we defined

$$\begin{aligned} \bar{\gamma}^{ij} & \equiv \frac{\gamma^{ij}}{\sqrt{m_i m_j \nu_i \nu_j}}, & \bar{\tau}^{ij} & \equiv \frac{\tau^{ij}}{\sqrt{m_i m_j \nu_i \nu_j}}, \\ \alpha_i & \equiv \ln \sqrt{m_i \nu_i}, \end{aligned}$$

from which one derives the equations of motion as

$$\dot{\theta}_i = \frac{\partial \mathcal{H}}{\partial I_i} \quad \text{and} \quad \dot{I}_i = -\frac{\partial \mathcal{H}}{\partial \theta_i}. \quad (131)$$

That this form of the Hamiltonian does not lead to divergent behavior of the  $\beta$  functions as discussed below Eq. (103) has been proven in Ref. [21] for the single component case. It also works for the  $N$ -fluids case, as we show below.

### C. Ultraviolet Behavior

Let us now discuss the UV expansion of the solutions of the Hamiltonian (125). We want to show that a particular choice of initial conditions renders the respective  $\beta$  functions such that the particle number densities remain finite at all times. Arguably, this choice of initial conditions provides a natural and well-defined vacuum which generalizes the single-field case.

Let us begin by working out the spectral dependence of the various terms involved in the UV limit  $\lambda_{\mathbf{k}} \rightarrow \infty$ . We are dealing with general Hamiltonians of the form (104), which we want to compare with the specific case of Eq. (74). We find that the kinetic matrix  $\mathsf{T}$  depends on the Laplacian only through  $\Delta_K$ , and this, in the UV limit, is simply the identity. This means that the asymptotic behavior of the kinetic matrix is  $\lim_{\lambda_{\mathbf{k}} \rightarrow \infty} \mathsf{T} = \mathcal{O}(\lambda_{\mathbf{k}}^0)$ . It is also easy to see that for a set of scalar fields with canonical kinetic terms this matrix will not depend on the Laplacian. For these reasons, we will focus our attention to the case where  $\lim_{\lambda_{\mathbf{k}} \rightarrow \infty} \mathsf{T} = \mathcal{O}(\lambda_{\mathbf{k}}^0)$ . It is worth emphasizing that such a behavior encompasses a large class of kinetic terms. Similarly, the potential matrix in Eq. (74) leads to terms proportional to the Laplacian, so that its expected behavior in the UV limit is  $\mathcal{O}(\lambda_{\mathbf{k}}^2)$ . Again the same spectral dependence is found in the case of a set of scalar fields whose couplings do not depend on spatial derivatives. Hence, we will focus on the case where  $\lim_{\lambda_{\mathbf{k}} \rightarrow \infty} \mathsf{V} = \mathcal{O}(\lambda_{\mathbf{k}}^2)$ .

Using Eqs. (111) and (112), we have that the normalization condition  $Q^{ia} \Pi_a^j = i\delta^{ij}$  translates into

$$q^j \mathsf{T}^{-1} q^j = 1. \quad (132)$$

Assuming the Hamiltonian to be ghost-free, the matrix  $\mathsf{T}$  must be positive definite. In this case, the asymptotic behavior of the vector  $q^j$  is  $\lim_{\lambda_{\mathbf{k}} \rightarrow \infty} q^j = \mathcal{O}(\lambda_{\mathbf{k}}^0)$ . From these UV behaviors, we conclude from Eq. (109) that

$$\lim_{\lambda_{\mathbf{k}} \rightarrow \infty} \nu_i = \mathcal{O}(\lambda_{\mathbf{k}})$$

and, from Eqs. (119), (126) and (127), we get

$$\lim_{\lambda_{\mathbf{k}} \rightarrow \infty} \mathcal{M}^{ij} = \mathcal{O}(\lambda_{\mathbf{k}}^0), \quad \lim_{\lambda_{\mathbf{k}} \rightarrow \infty} \bar{\gamma}^{ij} = \mathcal{O}(\lambda_{\mathbf{k}}^{-1}),$$

$$\lim_{\lambda_{\mathbf{k}} \rightarrow \infty} \bar{\tau}^{ij} = \mathcal{O}(\lambda_{\mathbf{k}}^0).$$

Finally, we can make use of our freedom in choosing  $m_i$ ,<sup>4</sup> to ensure that

$$\lim_{\lambda_{\mathbf{k}} \rightarrow \infty} \dot{\alpha}_i = \mathcal{O}(\lambda_{\mathbf{k}}^{-2}).$$

Since we are using  $\nu_i$  instead of  $\bar{\nu}_i$ , one can see that for the fluid Hamiltonian Eqs. (74–76), the frequencies  $\nu_i^2$  are built from a time dependent function times the Laplacian. In this case, we can choose  $m_i$  to cancel out this time dependent function and provides  $m_i \nu_i = \lambda_{\mathbf{k}}$ , and, consequently  $\dot{\alpha}_i = 0$ . In our asymptotic analysis, we are always considering the worst possible behavior (largest power of  $\lambda_{\mathbf{k}}$ ) of the variables involved. This will be, in turn, enough to show that particle production is well-behaved. Once we know the asymptotic behavior of every term in the Hamiltonian tensor Eq. (130) in the UV limit, we can work out the required initial conditions.

Since we construct our variables from the Hamiltonian tensor eigenvectors, all terms in Eq. (130) only depend on time derivatives of the original Hamiltonian tensor components  $\mathcal{H}^{ab}$ . This means that even if the original Hamiltonian contains strong couplings between the fields, the coefficients in Eq. (130) will be small as long as the Hamiltonian tensor itself varies adiabatically compared with the mode evolution. Let us introduce an “adiabatic parameter”  $\epsilon$  in the time derivative, i.e.,  $\mathcal{L}_{\bar{u}} \rightarrow \epsilon \mathcal{L}_{\bar{u}}$ , such that every time derivative of  $\mathcal{H}^{ab}$  produces a factor of  $\epsilon$ . Consequently, the quantities  $\dot{\alpha}_i$  and  $\bar{\tau}^{ij}$  are all at least first order in  $\epsilon$ , and  $\bar{\gamma}^{ij}$  is at least of second order [Eq. (126)]. One can observe that  $\bar{\gamma}^{ij}$ , which plays the role of the potential in the single component case, behaves as a second order adiabatic quantity, while the coupling  $\bar{\tau}^{ij}$  is a first order adiabatic quantity introduced by our first canonical transformation which is only present in the many component case.

The equations of motion (131) yield, for the angles,

$$\dot{\theta}_i = \nu_i + \dot{\alpha}_i \sin(2\theta_i) - \bar{\gamma}^{ii} \sin(\theta_i)^2 - \frac{\mathcal{F}_i}{\sqrt{I_i}}, \quad (133)$$

where

$$\mathcal{F}_i \equiv \sum_{j \neq i} \sqrt{I_j} \left[ \sin \theta_i \sin \theta_j \bar{\gamma}^{ij} + \frac{\sin(\theta_i - \theta_j) \bar{\tau}^{ij}}{2} \right]. \quad (134)$$

The adiabatic invariants  $I_i$  then satisfy

$$\dot{I}_i = [\sin(2\theta_i) \bar{\gamma}^{ii} - 2\dot{\alpha}_i \cos(2\theta_i)] I_i$$

$$+ \sum_{j \neq i} \sqrt{I_i I_j} [2 \cos(\theta_i) \sin(\theta_j) \bar{\gamma}^{ij} + \cos(\theta_i - \theta_j) \bar{\tau}^{ij}]. \quad (135)$$

This set of equations potentially induces a technical difficulty. We need a complete set of linearly independent solutions to construct all necessary annihilation and creation operators [Eq. (95)]. Since the coupling terms are all at least of order  $\epsilon$ , then at zeroth order, the adiabatic invariants are all constant [Eq. (135)]. It is tempting to choose each solution such that only the  $\ell^{\text{th}}$  adiabatic invariant is not vanishing at this order. This choice produces a set of operators such that when setting  $\epsilon \rightarrow 0$ , we obtain that each creation/annihilation only affects the  $\ell^{\text{th}}$  field variable. In short, for the  $\ell^{\text{th}}$  solution, all other adiabatic invariants  $i \neq \ell$  are at least of order  $\epsilon$ . The problem appears when we plug our solutions for  $I_i$  back into the equations of motion for the angles. In this case the presence of the factor  $I_i^{-1/2}$  in Eq. (133) turns these terms into zeroth order terms too. As a consequence, these equations for the angles no longer decouple at this lowest order. We will see below that this zeroth order term is actually signaling that the subsidiary modes  $i \neq \ell$  frequencies are indeed modified at zeroth order.

We can circumvent this problem by introducing a new set of variables representing the adiabatic invariant “square-root”, namely the complex fields  $A_{\ell i}$  satisfying

$$A_{\ell i} A_{\ell i}^* = I_{\ell i}, \quad (136)$$

keeping in mind that these complex variables are not to be understood as complexified solutions for the field, but merely a convenient form to express the adiabatic expansion, i.e.,  $A_{\ell i} \equiv \sqrt{I_{\ell i}} e^{i\theta_{\ell i}}$ . We also introduced the first index in the variables above to label the solution, i.e., the first index specifies the solution and the second the phase space component. This scheme will be maintained from here on. The equations of motion for these variables are

$$\dot{A}_{\ell i} = i \left( \nu_i - \frac{\bar{\gamma}^{ii}}{2} \right) A_{\ell i} + \left( \frac{i \bar{\gamma}^{ii}}{2} - \dot{\alpha}_i \right) A_{\ell i}^*$$

$$+ \frac{1}{2} \sum_{j \neq i} [(\bar{\tau}^{ij} - i \bar{\gamma}^{ij}) A_{\ell j} + i \bar{\gamma}^{ij} A_{\ell j}^*]. \quad (137)$$

The effective frequency appearing in the first term of the equation above can easily be identified as the first order expansion of the frequency defined in Eq. (128), i.e.,

$$\bar{\nu}_i = \nu_i - \frac{1}{2} \bar{\gamma}^{ii} + \mathcal{O}(\lambda_{\mathbf{k}}^{-2}).$$

Our choice of using the frequency  $\nu_i$  instead of  $\bar{\nu}_i$  makes the solutions differ at the order  $\mathcal{O}(\lambda_{\mathbf{k}}^{-2})$ . This is a convenient choice for our purpose since it simplifies the coupling term  $\bar{\tau}^{ij}$  while not spoiling the convergence requirements.

Defining the angle variable

$$\sigma_i = \int_{t_0}^t dt \left( \nu_i - \frac{1}{2} \bar{\gamma}^{ii} \right), \quad (138)$$

<sup>4</sup> See [21] for a detailed discussion about this point.

we rewrite the equations of motion as

$$\begin{aligned} \dot{B}_{\ell i} = & \left( \frac{i\bar{\gamma}^{ii}}{2} - \dot{\alpha}_i \right) e^{-2i\sigma_i} B_{\ell i}^* \\ & + \frac{1}{2} e^{-i\sigma_i} \sum_{j \neq i} [(\bar{\tau}^{ij} - i\bar{\gamma}^{ij}) e^{i\sigma_j} B_{\ell j} + i\bar{\gamma}^{ij} e^{-i\sigma_j} B_{\ell j}^*], \end{aligned} \quad (139)$$

where  $B_{\ell i} \equiv e^{-i\sigma_i} A_{\ell i}$ . We can now write the adiabatic expansion as

$$B_{\ell i} = \sum_{n=0}^{\infty} B_{\ell i}^{(n)}, \quad (140)$$

where  $B_{\ell i}^{(n)}$  is of order  $\mathcal{O}(\epsilon^n)$ . At zeroth order, the equation of motion is seen to reduce to

$$\dot{B}_{\ell i}^{(0)} = 0, \quad (141)$$

whose solutions are constants, i.e., each mode oscillates with its natural frequency through  $\sigma_i$  at first order in  $\epsilon$ . As discussed above, we may choose  $B_{\ell i}^{(0)}(t_0) = 0$  for all  $i \neq \ell$  to obtain the  $\ell^{\text{th}}$  solution and  $B_{\ell \ell}^{(0)}(t_0) = a_\ell$ , for an arbitrary complex constant  $a_\ell$ . For this reason, we need to go to the next order to obtain the spectral dependency of the subsidiary modes  $i \neq \ell$ .

The equations at first order can be split into an equation for the phase space component  $\ell$ ,<sup>5</sup>

$$\dot{B}_{\ell \ell}^{(1)} = \left( \frac{i}{2} \bar{\gamma}^{\ell \ell} - \dot{\alpha}_\ell \right) e^{-2i\sigma_\ell} a_\ell^*, \quad (142)$$

and another for  $i \neq \ell$

$$\dot{B}_{\ell i}^{(1)} = \frac{1}{2} e^{-i\sigma_i} [(\bar{\tau}^{i\ell} - i\bar{\gamma}^{i\ell}) e^{i\sigma_\ell} a_\ell + i\bar{\gamma}^{i\ell} e^{-i\sigma_\ell} a_\ell^*]. \quad (143)$$

Equation (142) can be solved by quadrature, i.e.,

$$B_{\ell \ell}^{(1)} = B_{\ell \ell}^{(1)}(t_0) + a_\ell^* \int_{t_0}^t dt \left( \frac{i}{2} \bar{\gamma}^{\ell \ell} - \dot{\alpha}_\ell \right) e^{-2i\sigma_\ell}, \quad (144)$$

which, once integrated by parts, leads to

$$B_{\ell \ell}^{(1)} = ia_\ell^* \left( \frac{i}{2} \bar{\gamma}^{\ell \ell} - \dot{\alpha}_\ell \right) \frac{e^{-2i\sigma_\ell}}{2\dot{\sigma}_\ell}. \quad (145)$$

The other terms are proportional to time derivatives of the coupling variables, and consequently are of higher order in the adiabatic expansion. We can also use the freedom in choosing  $B_{\ell \ell}^{(1)}(t_0)$  to cancel out the contribution of the integration by parts at  $t_0$ . Such a choice is justified since it is the only one for which  $B_{\ell \ell}^{(1)}$  goes

to zero when evaluated at a time at which the coupling goes to zero. Equation (145) shows that the first adiabatic correction to the principal phase space variable  $\ell$  is of order  $\mathcal{O}(\lambda_{\mathbf{k}}^{-2})$  in the UV limit.

A similar calculation for  $i \neq \ell$  [Eq. (143)] results in

$$B_{\ell i}^{(1)} = \frac{1}{2} e^{-i\sigma_i} \left( \frac{i\bar{\tau}^{i\ell} + \bar{\gamma}^{i\ell}}{\dot{\sigma}_i - \dot{\sigma}_\ell} e^{i\sigma_\ell} a_\ell - \frac{\bar{\gamma}^{i\ell} e^{-i\sigma_\ell}}{\dot{\sigma}_i + \dot{\sigma}_\ell} a_\ell^* \right). \quad (146)$$

Evaluating the UV limit, we obtain that  $B_{\ell i}^{(1)}$  is of order  $\mathcal{O}(\lambda_{\mathbf{k}}^{-1})$ . Finally, moving back to the original  $A_i$ , we get

$$\begin{aligned} A_{\ell \ell} &= a_\ell e^{i\sigma_i} + ia_\ell^* \left( \frac{i}{2} \bar{\gamma}^{\ell \ell} - \dot{\alpha}_\ell \right) \frac{e^{-i\sigma_\ell}}{2\dot{\sigma}_\ell} + \mathcal{O}(\epsilon^2), \\ A_{\ell i} &= \frac{1}{2} \left( \frac{i\bar{\tau}^{i\ell} + \bar{\gamma}^{i\ell}}{\dot{\sigma}_i - \dot{\sigma}_\ell} e^{i\sigma_\ell} a_\ell - \frac{\bar{\gamma}^{i\ell} e^{-i\sigma_\ell}}{\dot{\sigma}_i + \dot{\sigma}_\ell} a_\ell^* \right) + \mathcal{O}(\epsilon^2). \end{aligned}$$

Our choice of initial conditions makes the subsidiary modes oscillate with the same frequency as the principal mode  $\ell$ . Moreover, the mode  $A_{\ell i}$  oscillates with both positive and negative frequencies  $\dot{\sigma}_\ell$ . This behavior explains why the equation of motion for the angle  $\theta_{\ell i}$  is modified at zeroth order.

The equations above provide  $N$  real solutions for our system of equations. To form a complete set, we need  $2N$  real solutions which we use to build the  $N$  complex phase space vectors  $\mathbf{T}_a^i$  presented in (89). Given two real set of solutions  $(Q_{\ell i}^{\text{Re}}, P_{\ell i}^{\text{Re}})$  and  $(Q_{\ell i}^{\text{Im}}, P_{\ell i}^{\text{Im}})$ ,<sup>6</sup> we can write a complex set through

$$\begin{aligned} \mathbf{T}_i^\ell &= \frac{1}{2} [Q_{\ell i}^{\text{Re}}(I_{\ell i}^{\text{Re}}, \theta_{\ell i}^{\text{Re}}) - iQ_{\ell i}^{\text{Im}}(I_{\ell i}^{\text{Re}}, \theta_{\ell i}^{\text{Re}})], \\ \mathbf{T}_{i+N}^\ell &= \frac{1}{2} [P_{\ell i}^{\text{Re}}(I_{\ell i}^{\text{Re}}, \theta_{\ell i}^{\text{Re}}) - iP_{\ell i}^{\text{Im}}(I_{\ell i}^{\text{Im}}, \theta_{\ell i}^{\text{Im}})]. \end{aligned}$$

Each solution has its own adiabatic invariant and angle, i.e.,  $(I_i^{\text{Re}}, \theta_i^{\text{Re}})$  and  $(I_i^{\text{Im}}, \theta_i^{\text{Im}})$ , respectively, for the solutions playing the roles of the real and imaginary part. Note that, for the real part, we use a different parametrization than that given in Eq. (129), shifting the angle by  $\pi/2$ , as discussed in [21], i.e.,

$$Q_{\ell i}^{\text{Re}} = \frac{\sqrt{2I_{\ell i}^{\text{Re}}}}{e^{\alpha_i}} \cos \theta_{\ell i}^{\text{Re}}, \quad P_{\ell i}^{\text{Re}} = -e^{\alpha_i} \sqrt{2I_{\ell i}^{\text{Re}}} \sin \theta_{\ell i}^{\text{Re}}, \quad (147)$$

$$Q_{\ell i}^{\text{Im}} = \frac{\sqrt{2I_{\ell i}^{\text{Im}}}}{e^{\alpha_i}} \sin \theta_{\ell i}^{\text{Im}}, \quad P_{\ell i}^{\text{Im}} = e^{\alpha_i} \sqrt{2I_{\ell i}^{\text{Im}}} \cos \theta_{\ell i}^{\text{Im}}. \quad (148)$$

In the limit  $\epsilon \rightarrow 0$  the adiabatic invariants are constant and the angles evolve solely with their respective frequency  $\nu_i$ . In that case, if we set the same initial

<sup>5</sup> In the following expressions we are keeping also second order adiabatic terms together with the first order ones for convenience.

<sup>6</sup> These variables should not be confused with the Hamiltonian tensor eigenvectors given through Eqs. (111) and (112).



conditions for the angles, they will remain equal, i.e.,  $\theta_{\ell i}^{\text{Re}} = \theta_{\ell i}^{\text{Im}}$  and, since the adiabatic invariants are constant, we can choose

$$I_{\ell i}^{\text{Re}} = I_{\ell i}^{\text{Im}} = \delta_{\ell i},$$

yielding

$$\mathbb{T}_{\ell}^{\ell} = \frac{e^{-\alpha_i - i\theta_{\ell i}^{\text{Re}}}}{\sqrt{2}} \delta_{\ell i}, \quad \mathbb{T}_{\ell+N}^{\ell} = -i \frac{e^{\alpha_i - i\theta_{\ell i}^{\text{Re}}}}{\sqrt{2}} \delta_{\ell i}. \quad (149)$$

In this case, in the solution  $\ell$  only the  $\ell^{\text{th}}$  variable and its momentum  $[(\ell+N)^{\text{th}}$  component] are different from zero, and this set clearly satisfies Eq. (95). This amounts to showing that our choice of parametrization [Eqs. (147) and (148)] with identical initial conditions for the real and imaginary parts results in the usual positive frequency solution for the decoupled system.

It is a simple matter to obtain the shifted version of the equations of motion using the new variables: setting

$$I_{\ell i}^{\text{Re}} = C_{\ell i}^* C_{\ell i}, \quad I_{\ell i}^{\text{Im}} = A_{\ell i}^* A_{\ell i},$$

the choice  $C_{\ell i} = A_i e^{i\pi/2}$  yields a modified version of Eq. (137), namely

$$\begin{aligned} \dot{C}_{\ell i} = & i \left( \nu_i - \frac{1}{2} \bar{\gamma}^{ii} \right) C_{\ell i} - \left( \frac{i}{2} \bar{\gamma}^{ii} - \dot{\alpha}_i \right) C_{\ell i}^* \\ & + \frac{1}{2} \sum_{j \neq i} [(\bar{\gamma}^{ij} - i\bar{\gamma}^{ij}) C_{\ell j} - i\bar{\gamma}^{ij} C_{\ell j}^*]. \end{aligned} \quad (150)$$

The only difference is the sign in front of the terms where the complex conjugate of the field appears. As was done for  $A_{\ell i}$ , a similar calculation can be performed, yielding

$$\begin{aligned} C_{\ell \ell} &= c_{\ell} e^{i\sigma_{\ell}} - i c_{\ell}^* \left( \frac{i}{2} \bar{\gamma}^{\ell \ell} - \dot{\alpha}_{\ell} \right) \frac{e^{-i\sigma_{\ell}}}{2\dot{\sigma}_{\ell}} + \mathcal{O}(\epsilon^2), \\ C_{\ell i} &= \frac{1}{2} \left( \frac{i\bar{\gamma}^{i\ell} + \bar{\gamma}^{i\ell}}{\dot{\sigma}_i - \dot{\sigma}_{\ell}} e^{i\sigma_i} c_{\ell} + \frac{\bar{\gamma}^{i\ell} e^{-i\sigma_{\ell}}}{\dot{\sigma}_i + \dot{\sigma}_{\ell}} c_{\ell}^* \right) + \mathcal{O}(\epsilon^2), \end{aligned}$$

where  $c_{\ell}$  is an arbitrary complex constant.

From the approximate solutions  $C_{\ell i}$ , we can extract the real part of the solution and from  $A_i$  the imaginary. Setting  $c_{\ell} = a_{\ell}$ , we obtain that  $A_{\ell \ell}$  and  $C_{\ell \ell}$  coincide at zeroth order, and that their difference is of order  $\mathcal{O}(\lambda_{\mathbf{k}}^{-2})$ . The same will be true for their module and argument, i.e.,

$$\begin{aligned} \theta_{\ell \ell}^{\text{Re}} &= \theta_{\ell \ell}^{\text{Im}} + \mathcal{O}(\lambda_{\mathbf{k}}^{-2}), \\ I_{\ell \ell}^{\text{Re}} &= I_{\ell \ell}^{\text{Im}} + \mathcal{O}(\lambda_{\mathbf{k}}^{-2}). \end{aligned}$$

Consequently, for the principal mode we have

$$\mathbb{T}_{\ell}^{\ell} = e^{-\alpha_{\ell}} \left[ \frac{|a_{\ell}|}{\sqrt{2}} e^{-i\sigma_{\ell}} + \mathcal{O}(\lambda_{\mathbf{k}}^{-2}) \right], \quad (151)$$

$$\mathbb{T}_{\ell+N}^{\ell} = e^{\alpha_{\ell}} \left[ -i \frac{|a_{\ell}|}{\sqrt{2}} e^{-i\sigma_{\ell}} + \mathcal{O}(\lambda_{\mathbf{k}}^{-2}) \right], \quad (152)$$

where we chose  $a_{\ell}$  real for simplicity. Note also that  $a_{\ell}$  is a zeroth order quantity since it must be chosen in order

to have normalized states. Now, the subsidiary modes  $i \neq \ell$  are given by

$$\mathbb{T}_{\ell}^i = e^{-\alpha_i} \left[ i \frac{|\bar{\gamma}^{i\ell} a_{\ell}| e^{-i\sigma_{\ell}}}{\sqrt{2} |\dot{\sigma}_i - \dot{\sigma}_{\ell}|} + \mathcal{O}(\lambda_{\mathbf{k}}^{-2}) \right], \quad (153)$$

$$\mathbb{T}_{\ell+N}^i = e^{\alpha_i} \left[ \frac{|\bar{\gamma}^{i\ell} a_{\ell}| e^{-i\sigma_{\ell}}}{\sqrt{2} |\dot{\sigma}_i - \dot{\sigma}_{\ell}|} + \mathcal{O}(\lambda_{\mathbf{k}}^{-2}) \right]. \quad (154)$$

Here we kept only the term involving  $\bar{\gamma}^{i\ell}$ , this term being proportional to  $\mathcal{O}(\lambda_{\mathbf{k}}^0)$ , whereas the coupling  $\bar{\gamma}^{i\ell}$  is of order  $\mathcal{O}(\lambda_{\mathbf{k}}^{-1})$ , therefore contributing only in the next order in the UV expansion.

It is worth emphasizing that the explicit form of the coupling containing the coefficient  $\bar{\gamma}^{ij}$  in the Hamiltonian [Eq. (130)] is what generates the subsidiary solution term of order  $\mathcal{O}(\lambda_{\mathbf{k}}^{-1})$ . However, since this term does not couple  $A_{\ell i}$  with  $A_{\ell j}^*$  [Eq. (137)], it does not change when we shift the equations by  $\pi/2$  to obtain the equations of motion for  $C_{\ell i}$ . As a result, it creates an identical term in both the real and imaginary adiabatic invariants and angles at first order. In contrast,  $\bar{\gamma}^{ij}$  does not appear in such special form and, therefore, it couples  $A_{\ell i}$  with  $A_{\ell j}^*$  generating different factors [of order  $\mathcal{O}(\lambda_{\mathbf{k}}^{-2})$ ] in the real and imaginary solutions. This behavior of the coupling  $\bar{\gamma}^{ij}$  is essential to obtain a well defined particle production, and it is a consequence of our choice of  $R^{ij}$  given by Eqs. (123) and (124).

In short, the principal mode  $\mathbb{T}_{\ell}^{\ell}$  and its momentum  $\mathbb{T}_{\ell+N}^{\ell}$  are composed of a zeroth order  $[\mathcal{O}(\lambda_{\mathbf{k}}^0)]$  term oscillating with the same complex exponential plus second order  $[\mathcal{O}(\lambda_{\mathbf{k}}^{-2})]$  corrections. The subsidiary modes  $i \neq \ell$  and their momenta are composed of a first order term  $[\mathcal{O}(\lambda_{\mathbf{k}}^{-1})]$  oscillating with the same complex exponential plus second order terms  $[\mathcal{O}(\lambda_{\mathbf{k}}^{-2})]$ .

Given our choice of initial conditions for the adiabatic corrections discussed below Eq. (145), the subsidiary modes go to zero when evaluated at a time where the couplings also go to zero. This results in the solutions approaching Eq. (149) in this time limit.<sup>7</sup> Consequently, these solutions satisfy the conditions present in Eq. (95) in the limit, choosing  $a_{\ell} = 1$ . Thus, since the product is constant, it will satisfy the conditions for any time  $t$ . In other words, these solutions define a set of creation/annihilation operators with the required commutation relations where modes are statistically independent of each other.

Before moving forward, it is important to understand why quantization of Hamiltonian (55) + (65) in the original variables, i.e., the adiabatic plus entropy modes variable split, would not be well defined. Take, for example,

<sup>7</sup> If the couplings never vanish, it is always possible to choose the initial conditions for the adiabatic corrections such that the subsidiary modes are exactly zero at a given time. In this case, it is reasonable to choose the initial time as that at which the couplings are minimized.

the two fluid Hamiltonian of Eq. (74). The coupling between modes appears as a product of the momenta times a time dependent function of order  $\mathcal{O}(\lambda_{\mathbf{k}}^0)$ . When written in terms of the adiabatic invariants, each momentum will contribute a factor of  $\mathcal{O}(\lambda_{\mathbf{k}}^{1/2})$  [see Eq. (129)]. For this reason, the final coupling between adiabatic invariants will be of order  $\mathcal{O}(\lambda_{\mathbf{k}}^1)$ . If the original coupling between momenta is small in a given time limit, one can perform the expansion in powers of the coupling as we have done for the adiabatic parameter. On the other hand, in this case, the subsidiary term is proportional to the coupling times a factor of order  $\mathcal{O}(\lambda_{\mathbf{k}}^1)$ . Now, applying the limit where the coupling goes to zero, we obtain the vacuum commonly used in the literature. However, since this term is also proportional to  $\mathcal{O}(\lambda_{\mathbf{k}}^1)$ , if we first perform the limit  $\lambda_{\mathbf{k}} \rightarrow \infty$ , we obtain infinity, violating the assumption that the coupling is small. Put in another way, the decoupling limit and the UV limit do not commute for this choice. Given small but finite couplings, there will always be an infinite range of UV modes where the small coupling approximation is not valid, so that such a vacuum definition is not UV complete. In contrast, our choice of variables generates couplings between the adiabatic invariants that are at most of order  $\mathcal{O}(\lambda_{\mathbf{k}}^0)$ . Therefore, in our case, the adiabatic and UV limits commute and a well-defined vacuum can be calculated for all UV modes.

The original form (47) provides a well-defined next-to-leading order approximation, yet it leads to a non-unitary evolution. The adiabatic/entropy split, leading naturally to the Hamiltonian (55) + (65), would seem to be even more problematic at first sight since it not only leads to a non-unitary evolution but actually has an ill-defined next-to-leading order approximation for the base functions.

In practice however, it turns out to be more convenient since it is in a block-diagonal form and thus easier to transform into the final, well-defined choice of variables with Hamiltonian (125), for which the evolution is unitary. Indeed, the coupling terms in (47) between the field variable and momenta do not satisfy the required symmetries. Therefore, they mix  $A_{\ell i}$  and  $A_{\ell i}^*$  at order  $\mathcal{O}(\lambda_{\mathbf{k}}^{-1})$  such that the subsidiary terms of this order no longer have equal real and imaginary adiabatic invariants and angles. Consequently, the presence of such terms generates a  $\mathcal{O}(\lambda_{\mathbf{k}}^{-1})$  term in the particle creation operator, which would thus not converge.

With the variables leading to (125), the leading approximation is given by Eqs. (151–154), so that every basis function for the  $\ell$  mode oscillates with the same frequency  $\sigma_\ell$ . In (47), the effective coupling  $\bar{\tau}^{ij}$  is not antisymmetric, and therefore the above-mentioned subsidiary terms would depend on both  $e^{-i\sigma_i}$  and  $e^{i\sigma_i}$ , thereby mixing positive and negative frequencies at leading order. This indicates particle creation at  $\mathcal{O}(\lambda_{\mathbf{k}}^{-1})$  order, and hence, the non unitary evolution advertised above. Ideally, the adiabatic/entropy intermediary mode expansion could be avoided by means of a direct trans-

formation from (47) to (125); in general however, going through this step provided a straightforward method to transform any block-diagonal Hamiltonian into the required form.

We are now in a position to evaluate whether the  $\beta^{ij}(t)$  calculated through Eq. (101) present the required convergent UV behavior, thereby providing acceptable initial conditions for a vacuum state. From Eq. (101), one obtains  $\beta^{ij}(t) = \mathbf{T}_a^i(t) \mathbf{t}^j_a$ , or, more explicitly,

$$\beta^{ij} = i \sum_r (\mathbf{T}_r^i \mathbf{t}_{r+N}^j - \mathbf{T}_{r+N}^i \mathbf{t}_r^j). \quad (155)$$

Each term of this expansion of  $\beta^{ij}$  depends on the factor of  $e^{\alpha_i - \alpha_i(t_0)}$ . This is exactly the problematic factor present in the single component quantization, discussed thoroughly in Ref. [21]. There it was shown that our choice of  $m_i$  is enough to make this factor behave as  $e^{\alpha_i - \alpha_i(t_0)} = 1 + \mathcal{O}(\lambda_{\mathbf{k}}^{-2})$ . These factors lead to convergent integrals and therefore can be safely ignored. Finally, for every mode, the leading term is symmetric when changing the time dependence, i.e.,

$$\mathbf{T}_r^i \mathbf{t}_{r+N}^j = \mathbf{t}_r^i \mathbf{T}_{r+N}^j + \mathcal{O}(\lambda_{\mathbf{k}}^{-2}),$$

and consequently, every term in the sum defining  $\beta^{ij}$  will be at least of order  $\mathcal{O}(\lambda_{\mathbf{k}}^{-2})$ . This amounts to showing that, for this choice of initial conditions and variables, the particle number density will be finite at all times and, therefore, that the time evolution of the quantum field operators will be unitary.

We stress at this point that it is not the leading order that would produce the divergent contribution for the particle creation, but the next-to-leading order: the leading order can be made to cancel out by an appropriate choice of the arbitrary mass functions appearing in Eqs. (111) and (112), but then the problem reappears at the following order for which no such arbitrarily adjustable functions is available. We also observe that is not necessary that all adiabatic corrections be of order  $\mathcal{O}(\lambda_{\mathbf{k}}^{-2})$ : if it was indeed the case, the term  $\bar{\tau}^{ij}$  would have spoiled the convergence. What is however necessary is that any coupling mixing  $A_{\ell i}$  and  $A_{\ell i}^*$  (consequently also  $C_{\ell i}$  and  $C_{\ell i}^*$ ) frequencies must be at least of order  $\mathcal{O}(\lambda_{\mathbf{k}}^{-2})$ . We have thus achieved our goal to obtain a consistent set of initial conditions leading to an unambiguous vacuum.

#### IV. CONCLUSION

Setting consistent and natural initial conditions for cosmological perturbations crucially depends on the model one is investigating. In inflationary models, very short wavelengths, i.e., those much smaller than the almost-constant Hubble scale, can always be seen as effectively evolving in a Minkowski universe, and can thus be given a natural vacuum initial state (or any other state one wishes [46]). Nonetheless, even in this case, not all canonical variables lead to a unitary evolution of

the quantum field, as was elucidated in [21]. In more complicated situations involving many fluids, things are worse, as the presence of subdominant modes creates new possibilities for divergences in the particle production. The present work goes one step further in completing the analysis by clarifying the situation when many components are present.

In the first part of this work, we managed to obtain the Hamiltonian for a set of fluids coupled only through gravitation. This Hamiltonian was obtained without ever using the background equations of motion. For this reason, one can use it even when the background is also quantized (see [2, 3] for a single fluid example) or in other settings where the background does not satisfy the classical equations of motion; another example is when the background is described by an averaged metric. One should also stress that the ambiguity in defining the gauge invariant perturbations discussed in [19] is also present in the many fluids case, so that our formalism is necessary to define the gauge invariant perturbation whenever one uses a nonclassical background.

The second part consists in establishing the general procedure for many component quantization. We restricted attention to cases where the original Hamiltonian tensor can be written in the form (104) and the spectral behavior of its many components described in Sec. III C. This restriction is however quite mild, as this encompasses most systems found in the literature. We showed that the usual procedure through which one determines the vacuum by expanding the solutions in terms of the original couplings is potentially ill defined. For example, if the original coupling terms appear as products of the different component momenta in the Hamiltonian, then the basis determination is incomplete in the UV limit, i.e., there always exists a value of  $\lambda_k$  beyond which the coupling becomes strong and the whole approximation invalid. Consequently, the UV limit does not commute

with the small coupling limit. This shows that determining the basis functions for quantization of multiple component systems using only the adiabatic expansion (or slow-roll approximation in a multifield inflation scenario) can be misleading since the corrections can have a divergent UV limit. In addition, we proved that with our choice of variables, the time evolution can be implemented by a unitary operator. This result extends the literature [21–33] by introducing for the first time a set of special canonical variables for a multiple component system coupled by quadratic terms in the Hamiltonian for which the time evolution is unitary. All these results were accomplished using adiabatic invariants, which proved essential to understand the UV asymptotic behavior of the solutions.

Our formalism can in particular be applied to the special case where only two fluids are present, in which case one needs not specify a privileged fluid with respect to which the other would be defined. Instead, one expands in the usual adiabatic and entropy modes, for which one then finds very natural vacuum (or else) initial conditions, where the quantum evolution is unitary. One can apply straightforwardly our result to specific cases involving, for instance, two fluids in a contracting and bouncing universe. That will be the subject of a subsequent work [47].

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- [1] F. Finelli and R. Brandenberger, *Phys. Rev. D* **65**, 103522 (2002), hep-th/0112249v2.
  - [2] P. Peter, E. J. C. Pinho, and N. Pinto-Neto, *Phys. Rev. D* **75**, 023516 (2007), arXiv:hep-th/0610205 [hep-th].
  - [3] P. Peter and N. Pinto-Neto, *Phys. Rev. D* **78**, 063506 (2008), arXiv:0809.2022 [gr-qc].
  - [4] J. Khoury, B. Ovrut, P. Steinhardt, and N. Turok, *Phys. Rev. D* **64**, 123522 (2001), hep-th/0103239v3.
  - [5] R. Kallosh, L. Kofman, and A. D. Linde, *Phys. Rev. D* **64**, 123523 (2001), arXiv:hep-th/0104073 [hep-th].
  - [6] J. Khoury, B. A. Ovrut, P. J. Steinhardt, and N. Turok, *Phys. Rev. D* **66**, 046005 (2002), arXiv:hep-th/0109050.
  - [7] J. Martin, P. Peter, N. Pinto-Neto, and D. J. Schwarz, *Phys. Rev. D* **65**, 123513 (2002), arXiv:hep-th/0112128.
  - [8] J. Martin, C. Ringeval, R. Trotta, and V. Vennin, *J. Cosmol. Astropart. Phys.* **1403**, 039 (2014), arXiv:1312.3529 [astro-ph.CO].
  - [9] C. T. Byrnes and D. Wands, *Phys. Rev. D* **74**, 043529 (2006), astro-ph/0605679.
  - [10] Z. Lalak, D. Langlois, S. Pokorski, and K. Turzyński, *J. Cosmol. Astropart. Phys.* **7**, 014 (2007), arXiv:0704.0212 [hep-th].
  - [11] D. Langlois and S. Renaux-Petel, *J. Cosmol. Astropart. Phys.* **4**, 17 (2008), arXiv:0801.1085 [hep-th].
  - [12] D. Langlois, S. Renaux-Petel, D. A. Steer, and T. Tanaka, *Phys. Rev. D* **78**, 063523 (2008), arXiv:0806.0336 [hep-th].
  - [13] D. Battefeld, T. Battefeld, C. Byrnes, and D. Langlois, *J. Cosmol. Astropart. Phys.* **8**, 025 (2011), arXiv:1106.1891 [astro-ph.CO].
  - [14] J. Ellis, M. A. G. García, D. V. Nanopoulos, and K. A. Olive, *J. Cosmol. Astropart. Phys.* **8**, 044 (2014), arXiv:1405.0271 [hep-ph].
  - [15] L. McAllister, S. Renaux-Petel, and G. Xu, *J. Cosmol. Astropart. Phys.* **10**, 046 (2012), arXiv:1207.0317.
  - [16] S. Mizuno, R. Saito, and D. Langlois, *J. Cosmol. Astropart. Phys.* **11**, 032 (2014), arXiv:1405.4257 [hep-th].

- [17] S. Renaux-Petel and K. Turzyński, J. Cosmol. Astropart. Phys. **6**, 010 (2015), arXiv:1405.6195.
- [18] S. Renaux-Petel and K. Turzyński, ArXiv e-prints (2015), arXiv:1510.01281.
- [19] S. D. P. Viti, F. T. Falciano, and N. Pinto-Neto, Phys. Rev. D **87**, 103503 (2013), arXiv:1206.4374 [gr-qc].
- [20] F. T. Falciano, N. Pinto-Neto, and S. D. P. Viti, Phys. Rev. D **87**, 103514 (2013), arXiv:1305.4664 [astro-ph.CO].
- [21] S. D. P. Viti, ArXiv e-prints (2015), arXiv:1505.01541 [gr-qc].
- [22] C. G. Torre, Phys. Rev. D **66**, 084017 (2002), arXiv:gr-qc/0206083.
- [23] A. Corichi, J. Cortez, G. A. M. Marugán, and J. M. Velhinho, Class. Quantum Grav. **23**, 6301 (2006), arXiv:gr-qc/0607136.
- [24] J. Cortez, G. A. M. Marugán, and J. M. Velhinho, Phys. Rev. D **75**, 084027 (2007), arXiv:gr-qc/0702117.
- [25] A. Corichi, J. Cortez, G. A. Mena Marugán, and J. M. Velhinho, Phys. Rev. D **76**, 124031 (2007), arXiv:0710.0277.
- [26] J. Fernando Barbero G., D. G. Vergel, and E. J. S. Villaseñor, Class. Quantum Grav. **25**, 085002 (2008), arXiv:0711.1790.
- [27] D. G. Vergel and E. J. S. Villaseñor, Class. Quantum Grav. **25**, 145008 (2008).
- [28] J. Cortez, G. A. M. Marugán, J. Olmedo, and J. M. Velhinho, Class. Quantum Grav. **28**, 172001 (2011).
- [29] L. C. Gomar, J. Cortez, D. M.-d. Blas, G. A. M. Marugán, and J. M. Velhinho, J. Cosmol. Astropart. Phys. **2012**, 001 (2012).
- [30] J. Cortez, G. A. Mena Marugán, J. Olmedo, and J. M. Velhinho, Phys. Rev. D **86**, 104003 (2012), arXiv:1202.6330.
- [31] M. Fernández-Méndez, G. A. Mena Marugán, J. Olmedo, and J. M. Velhinho, Phys. Rev. D **85** (2012), 10.1103/physrevd.85.103525, arXiv:1203.2525 [gr-qc].
- [32] J. Cortez, D. M.-d. Blas, G. A. M. Marugán, and J. M. Velhinho, Class. Quantum Grav. **30**, 075015 (2013).
- [33] J. Cortez, G. A. Mena Marugán, and J. M. Velhinho, ArXiv e-prints (2015), arXiv:1509.06171 [gr-qc].
- [34] S. D. P. Viti and N. Pinto-Neto, Phys. Rev. D **85**, 023524 (2012), arXiv:1111.0888 [astro-ph.CO].
- [35] J. M. Stewart, Class. Quantum Grav. **7**, 1169 (1990).
- [36] V. F. Mukhanov, H. A. Feldman, and R. H. Brandenberger, Phys. Rep. **215**, 203 (1992).
- [37] L. Faddeev and R. Jackiw, Physical Review Letters **60**, 1692 (1988).
- [38] R. Jackiw, ArXiv e-prints (1993), hep-th/9306075.
- [39] N. D. Birrell and P. C. W. Davies, *Quantum Fields in Curved Space* (Cambridge University Press, 1982) p. 340.
- [40] R. Wald, *Quantum field theory in curved spacetime and black hole thermodynamics*, Chicago lectures in physics (University of Chicago Press, 1994).
- [41] S. Winitzki, Phys. Rev. D **72**, 104011 (2005), gr-qc/0510001v2.
- [42] L. E. Parker and D. J. Toms, *Quantum field theory in curved spacetime: Quantized Field and Gravity* (Cambridge University Press, 2009).
- [43] L. Parker, J. Phys. A: Math. Theor. **45**, 374023 (2012).
- [44] M. E. Peskin and D. V. Schroeder, *An Introduction to quantum field theory* (Addison-Wesley, 1995).
- [45] D. Langlois, S. Renaux-Petel, D. A. Steer, and T. Tanaka, Phys. Rev. **D78**, 063523 (2008), arXiv:0806.0336 [hep-th].
- [46] J. Martin, A. Riazuelo, and M. Sakellariadou, Phys. Rev. D **61**, 083518 (2000), arXiv:astro-ph/9904167 [astro-ph].
- [47] P. Peter, N. Pinto-Neto, and S. D. P. Viti, in preparation (2015).